

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of Date: May 15, 2008  
Applicants: Bednorz et al. Docket: YO987-074BZ  
Serial No.: 08/479,810 Group Art Unit: 1751  
Filed: June 7, 1995 Examiner: M. Kopec  
For: NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION  
Commissioner for Patents  
United States Patent and Trademark Office  
P.O. Box 1450  
Alexandria, VA 22313-1450

# **APPEAL BRIEF**

## **PART IX**

**CFR 37 § 41.37(c) (1) (ix)**

## **SECTION 1**

# VOLUME 4

## Part 4

## **BRIEF ATTACHMENTS P TO Z**

Respectfully submitted,

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**BRIEF ATTACHMENT P**

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**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT P**

# LANDOLT-BÖRNSTEIN

Numerical Data and Functional Relationships  
in Science and Technology

*New Series*

Editor in Chief: K.-H. Hellwege

Group III: Crystal and Solid State Physics

Volume 3  
Ferro- and Antiferroelectric Substances

by Toshio Mitsui and

R. Abe · Y. Furuhata · K. Gesi · T. Ikeda · K. Kawabe  
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Spirit

## II Data Oxides

### 1 Perovskite-type oxides

#### 1A Simple perovskite-type oxides

##### Nr. 1A-1 NaNbO<sub>3</sub>, Sodium niobate

a	It was reported by MATTIAS et al. in 1951 that NaNbO <sub>3</sub> was ferroelectric. CROSS et al., however, proved in 1955 that at room temperature it is not ferroelectric but antiferroelectric.						51M2																													
b	<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th>phase</th><th>V</th><th>IV</th><th>III*</th><th>II</th><th>I</th></tr> <tr> <th>state</th><th>F</th><th>A</th><th></th><th></th><th>P</th></tr> <tr> <th>crystal system</th><td>monoclinic</td><td>orthorhombic</td><td>pseudo-tetragonal</td><td>tetragonal</td><td>cubic</td></tr> <tr> <th>space group</th><td></td><td>Pbma<sup>a)</sup>-D<sub>2h</sub><sup>11</sup></td><td></td><td></td><td>Pm3m-O<sub>h</sub></td></tr> <tr> <th><math>\Theta^{**}</math></th><td>-200</td><td>354</td><td>562</td><td>640</td><td>°C</td></tr> </thead> </table>					phase	V	IV	III*	II	I	state	F	A			P	crystal system	monoclinic	orthorhombic	pseudo-tetragonal	tetragonal	cubic	space group		Pbma <sup>a)</sup> -D <sub>2h</sub> <sup>11</sup>			Pm3m-O <sub>h</sub>	$\Theta^{**}$	-200	354	562	640	°C	55C2
phase	V	IV	III*	II	I																															
state	F	A			P																															
crystal system	monoclinic	orthorhombic	pseudo-tetragonal	tetragonal	cubic																															
space group		Pbma <sup>a)</sup> -D <sub>2h</sub> <sup>11</sup>			Pm3m-O <sub>h</sub>																															
$\Theta^{**}$	-200	354	562	640	°C																															
	<p><math>P_s \parallel [001]</math> in phase V.            Phase IV: <math>a = 5.568 \text{ \AA} (\cong \sqrt{2}a_0)</math>, <math>b = 5.505 \text{ \AA} (\cong \sqrt{2}a_0)</math>, <math>c = 15.518 \text{ \AA} (\cong 4a_0)</math>, where <math>a_0</math> is the lattice constant of the cubic cell of phase I.            In phase IV (orthorhombic system) the longest edge of a unit cell is taken as the <math>c</math> axis (see Fig. 1). This system of the axes is adopted here. In Well and Megaw's analysis <math>b</math> and <math>c</math> axes were interchanged. The orthorhombic structure is also represented by a pseudomonoclinic unit cell (see Fig. 1), where <math>b' = c</math>, <math>a' = c'</math> (<math>\cong a_0</math>), <math>\beta' \cong \pi/2</math>.</p>						<sup>a)</sup> 61W2 58R3																													
	<p>2a Cooling method from a molten mixture of Na<sub>2</sub>CO<sub>3</sub>, Nb<sub>2</sub>O<sub>5</sub>, and NaF.</p>						51W1																													
3	<p>Crystal structure: In phase IV, <math>Z = 8</math>.            Tab. 1; Fig. 1, 2.</p>																																			
4	<p>Lattice distortions (thermal expansion): For phase I, II, III, IV: Tab. 2, 3; Fig. 3.            For phase V, at -160 °C: <math>a = 5.564 \text{ \AA} (\cong \sqrt{2}a_0)</math>, <math>b = 5.548 \text{ \AA} (\cong \sqrt{2}a_0)</math>, <math>c = 7.812 \text{ \AA} (\cong 2a_0)</math>, <math>\beta = 91^\circ 09'</math>.            Fig. 4.</p>						57J1																													
5a	<p>Dielectric constants: Fig. 5.            Curie-Weiss law: <math>\chi = C/(T - \Theta_p)</math>, <math>T &gt; \Theta_{III-IV}</math>, where <math>C = 2 \dots 4 \cdot 10^5 \text{ ^\circ K}</math> and <math>\Theta_p = 60 \dots 80 \text{ ^\circ C}</math>.</p>						54S3																													
c	<p>Spontaneous polarization: <math>P_s \cong 12 \cdot 10^{-8} \text{ C m}^{-2}</math> (<math>\parallel c</math>, in phase V).            Coercive and critical field for normal and double hysteresis curve: Fig. 6.</p>						55C2																													
9a	<p>Birefringence: Fig. 7, 8.</p>																																			
14a	<p>Domain structure: See</p>						<sup>55C2, 64p1,</sup> <sup>62M9, 62W3</sup>																													
b	<p>Dynamic properties: Fig. 9, 10.</p>																																			

Tab. 1. NaNbO<sub>3</sub>. Fractional coordinates  $x$ ,  $y$ ,  $z$  of atoms in unit cell at RT. [61W2]

	$x$	$y$	$z$
Na(1)	$\frac{1}{4}$	0.250	0
Na(2)	0.769	0.251	$\frac{1}{4}$
Nb	0.261	0.257	0.125
O(1)	$\frac{1}{4}$	0.208	0
O(2)	0.271	0.290	$\frac{1}{4}$
O(3)	0.010	0.532	0.121
O(4)	0.446	0.972	0.126

\* According to Ismailzade phase III consists of 4 phases (see Fig. 3). [63J4]  
 Transitions exhibit large temperature hysteresis, and the transition temperatures measured with decreasing temperature are given here.

## II 1 Oxide des Perowskit-Typs

Tab. 2.  $\text{NaNbO}_3$ . Lattice parameters at various temperatures. [56F1] and [54S3]

$T$ [°C]	Crystal symmetry	Lattice parameters	
		[56F1]	[54S3]
20	Monoclinic	$a' = c' = 3.914 \text{ \AA}$ $b' = 4 \cdot 3.881 \text{ \AA}$ $\beta' = 90^\circ 39'$	$a' = c' = 3.915 \text{ \AA}$ $b' = 4 \cdot 3.881 \text{ \AA}$ $\beta' = 90^\circ 40'$
390	Pseudotetragonal	$a = 2 \cdot 3.920 \text{ \AA}$ $c = 4 \cdot 3.926 \text{ \AA}$ $c/a = 2.0032$	$a = 2 \cdot 3.919 \text{ \AA}$ $c = 4 \cdot 3.927 \text{ \AA}$ $c/a = 2.0040$
420	Pseudotetragonal	$a = 2 \cdot 3.924 \text{ \AA}$ $c = 4 \cdot 3.924 \text{ \AA}$ $c/a \approx 2.0000$	$a = 2 \cdot 3.921 \text{ \AA}$ $c = 4 \cdot 3.927 \text{ \AA}$ $c/a = 2.0028$
560	Tetragonal (changing to simple perovskite-type cell)	$a = 2 \cdot 3.933 \text{ \AA}$ $c = 4 \cdot 3.940 \text{ \AA}$ $c/a = 2.0038$	—
640	Cubic	$a = 3.942 \text{ \AA}$	—

Tab. 3.  $\text{NaNbO}_3$ . Lattice parameters of the subcell at various temperatures. [63I4]. See Fig. 3

$T$ [°C]	Subcell parameters				
	pseudomonoclinic I ( $a' = c' > b'$ , $\beta' > 90^\circ$ )				
	$a'$ [\AA]	$b'$ [\AA]	$\beta' - 90^\circ$	$a'/b'$	$V$ [\AA <sup>3</sup> ]
18 ... 20	3.914 <sub>s</sub>	3.885	40'	1.0075 <sub>s</sub>	59.5 <sub>s</sub>
100	3.917	3.893 <sub>s</sub>	37	1.0060	59.7 <sub>s</sub>
150	3.919 <sub>s</sub>	3.898 <sub>s</sub>	33	1.0055	59.9
200	3.922 <sub>s</sub>	3.902 <sub>s</sub>	29	1.0050	60.0 <sub>s</sub>
250	3.924 <sub>s</sub>	3.907 <sub>s</sub>	26	1.0040	60.1 <sub>s</sub>
300	3.925 <sub>s</sub>	3.914	22	1.0030	60.3 <sub>s</sub>
340	3.926 <sub>s</sub>	3.917 <sub>s</sub>	18	1.0025	60.4
350	3.926 <sub>s</sub>	3.919	17	1.0020 <sub>s</sub>	60.4 <sub>s</sub>
pseudomonoclinic II					
360	3.927 <sub>s</sub>	3.920	6	1.0020	60.45
380	3.927 <sub>s</sub>	3.921 <sub>s</sub>	5	1.0015 <sub>s</sub>	60.50
400	3.928 <sub>s</sub>	3.922 <sub>s</sub>	4	1.0015	60.5 <sub>s</sub>
pseudomonoclinic III					
420	3.929 <sub>s</sub>	3.923	3	1.0015	60.5 <sub>s</sub>
440	3.930 <sub>s</sub>	3.924	3	1.0015	60.6 <sub>s</sub>
460	3.932	3.926 <sub>s</sub>	3	1.0015	60.70
pseudomonoclinic IV					
480	3.933 <sub>s</sub>	3.927 <sub>s</sub>	3	1.0015 <sub>s</sub>	60.7 <sub>s</sub>
500	3.934 <sub>s</sub>	3.928 <sub>s</sub>	2	1.0015 <sub>s</sub>	60.8 <sub>s</sub>
510	3.935	3.929 <sub>s</sub>	2	1.0015	60.85
tetragonal I					
$T$ [°C]	$c$ [\AA]	$a = b$ [\AA]	$c/a$	$V$ [\AA <sup>3</sup> ]	
520	3.936 <sub>s</sub>	3.929 <sub>s</sub>	1.0015 <sub>s</sub>	60.80	
540	3.938	3.930 <sub>s</sub>	1.0020	60.85	
560	3.939 <sub>s</sub>	3.931 <sub>s</sub>	1.0020 <sub>s</sub>	60.90	
tetragonal II					
580	3.941 <sub>s</sub>	3.934 <sub>s</sub>	1.0020	61.00	
600	3.943 <sub>s</sub>	3.937 <sub>s</sub>	1.0015	61.15	
620	3.945 <sub>s</sub>	3.942	1.0010	61.30	
630	3.945	$\approx 3.945$	$\approx 1.0000$	61.40	
cubic					
$T$ [°C]	$a_0$ [\AA]	$V$ [\AA <sup>3</sup> ]	$T$ [°C]	$a_0$ [\AA]	$V$ [\AA <sup>3</sup> ]
640	3.947 <sub>s</sub>	61.50	700	3.949 <sub>s</sub>	61.6 <sub>s</sub>
650	3.947 <sub>s</sub>	61.5 <sub>s</sub>	720	3.950 <sub>s</sub>	61.6 <sub>s</sub>
680	3.949	61.5 <sub>s</sub>			

Nr.

1a  
b

2

3

4

5

6

7

12

\* Nt

\*\* Fo

Nr. 1A-2 KNbO<sub>3</sub>, Potassium niobate

1a b	Ferroelectricity in KNbO <sub>3</sub> was first discovered by MATTHIAS in 1949.	49M4			
	phase	IV	III	II	I
	state	F	F	F	P
	crystal system	rhombohedral	orthorhombic	tetragonal	cubic
	space group		Bmm2 <sup>a</sup> )C <sub>2v</sub> <sup>16</sup>		Pm3m-O <sub>h</sub> <sup>1</sup>
	$\Theta$	-10	225	435	°C
	$P_s \parallel [001]$ in phase II (along [001] of phase I), $P_s \parallel [001]$ in phase III (along [110] of phase I), $P_s \parallel [111]$ in phase IV (along [111] of phase I). $T_{\text{melt}} = 1050$ °C $\epsilon = 4.590 \cdot 10^8$ kg m <sup>-3</sup> $a = 5.697$ Å, $b = 3.971$ Å, $c = 5.720$ Å at RT. Transparent. Light yellow.				
2	Flux method ( $K_2CO_3$ flux). Phase diagram of $K_2CO_3$ -Nb <sub>2</sub> O <sub>5</sub> system; see Pulling method from the $K_2CO_3$ -Nb <sub>2</sub> O <sub>5</sub> mixture Crystal form: square plate	51W1 55R3 58M3			
3	Crystal structure: $Z = 1$ in phase I, II, IV. $Z = 2$ in phase III. Tab. 4, 5; Fig. 11.				
4	Temperature dependence of lattice parameters: Tab. 6; Fig. 12.				
5	Dielectric constant: Fig. 13, 14. $\kappa = C/(T - \Theta_p)$ , $T > \Theta_{II-I}$ , where $C = 2.42 \cdot 10^5$ °K, $\Theta_p = 360$ °C. Nonlinear dielectric properties: $\xi = -1.62 \cdot 10^8$ J C <sup>-4</sup> m <sup>5</sup> , $\zeta = 1.79 \cdot 10^{10}$ J C <sup>-6</sup> m <sup>9</sup> . Spontaneous polarization and coercive field: Fig. 15. $P_s = 26 \cdot 10^{-2}$ C m <sup>-2</sup> at $T = \Theta_p$ .	56T3 56T3 56T3			
6	Transition heat, transition entropy: Tab. 7.	56T3			
7	Piezoelectricity: Fig. 16.				
12	NQR: Tab. 8; Fig. 17 ... 20.				

Tab. 4. KNbO<sub>3</sub>. Atomic positions in fractional coordinates at RT in phase III. [67K4]

Nb	0, 0, 0
K	0, $\frac{1}{2}$ , $\frac{1}{2} + z_K$
O(1)	0, $\frac{1}{2}$ , $z_1$
O(2)	$\frac{1}{2} + z_1$ , 0, $\frac{1}{2} + z_2$
$z_K$	+0.017
$z_1$	+0.021
$z_2$	+0.035
$z_2$	+0.004

Tab. 5. KNbO<sub>3</sub>. Interatomic distances and bond angles at RT. [67K4]

	*	distance Å	**	*	angle °
Nb-O(1)	(2)	$1.991 \pm 0.001$	O(2)(s)-Nb-O(2)(s)	(1)	$97.4 \pm 1.2$
Nb-O(2)	(2)	$1.863 \pm 0.007$	O(2)(l)-Nb-O(2)(l)	(1)	$83.4 \pm 1.0$
Nb-O(2)	(2)	$2.180 \pm 0.009$	O(2)(s)-Nb-O(2)(l)	(2)	$89.7 \pm 0.5$
K-O(1)	(1)	$2.837 \pm 0.014$	O(1)-Nb-O(2)(s)	(4)	$92.3 \pm 0.6$
K-O(1)	(2)	$2.848 \pm 0.001$	O(1)-Nb-O(2)(l)	(4)	$87.5 \pm 0.6$
K-O(1)	(1)	$2.883 \pm 0.014$	Nb-O(1)-Nb	(1)	$172.8 \pm 0.7$
K-O(2)	(4)	$2.792 \pm 0.008$	Nb-O(2)-Nb	(2)	$168.6 \pm 0.6$
K-O(2)	(4)	$2.873 \pm 0.010$			
O(1)-O(2)	(4)	$2.780 \pm 0.012$			
O(1)-O(2)	(4)	$2.884 \pm 0.012$			
O(2)-O(2)	(1)	$2.802 \pm 0.024$			
O(2)-O(2)	(1)	$2.894 \pm 0.024$			
O(2)-O(2)	(2)	$2.860 \pm 0.001$			

\* Numbers in this column indicate numbers of equal bonds or angles per formula unit.

For the O-Nb-O angles, the letter s or l indicates whether the Nb-O(2) bond involved is short or long.

Tab. 6. KNbO<sub>3</sub>. Lattice constants and volume of unit cell at various temperatures. [54S3].  $a'$ ,  $c'$ : lattice parameters of pseudotetragonal cell

$T$ °C	$a' = c'$ Å	$b$ Å	$b/a$	$\beta$	$V$ Å <sup>3</sup>
25	4.0375	3.9711	1.0167	90° 15'	64.73
125	4.0374	3.9797	1.0145	90° 15'	64.87
185	4.0363	3.9830	1.0134	90° 13'	64.89
205	4.0369	3.9839	1.0133	90° 14'	64.93
	$a = b$	$c$	$c/a$		
220	3.9972	4.0636	1.0166		64.92
230	3.9978	4.0640	1.0166		64.95
270	3.9992	4.0647	1.0164		65.01
320	4.0023	4.0639	1.0154		65.10
375	4.0048	4.0620	1.0143		65.15
410	4.0080	4.0567	1.0122		65.18
425	4.0214				65.03
450	4.0225				65.09
510	4.0252				65.22

Tab. 7. KNbO<sub>3</sub>. Transition heat and transition entropy per mole. [54S1]

Transition	$\Delta Q_m$ cal mol <sup>-1</sup>	$\Delta S_m$ cal °K <sup>-1</sup> mol <sup>-1</sup>
IV → III	32	0.12
III → II	85	0.17
II → I	190	0.28
	134	—

Tab. 8. KNbO<sub>3</sub>. NQR spectrum. [54C1]. The measured frequency ratios intersect the calculated ratios in a straight line at constant  $\eta = 0.806 \pm 0.002$ .  
 $\eta$  = asymmetry parameter

Crystal structure	$f$ MHz	Measured ratio	Calculated ratio ( $\eta = 0.806$ )	Identification	$e^2 q Q/h$ MHz
orthorhombic (20 °C)	3.648	1.204	1.204	(9/2, 7/2)	23.120 ± 0.05
	3.030	1.198	1.196	(3/2, 1/2)	
	2.527	1.214	1.213	(7/2, 5/2)	
	2.085			(5/2, 3/2)	
rhombohedral (-196 °C)	2.674		( $\eta = 0.0$ )		
	2.004	1.335	1.333	(9/2, 7/2)	16.0 ± 0.1
	1.335	1.503	1.500	(7/2, 5/2)	
				(5/2, 3/2)	

### Nr. 1A-3 NaTaO<sub>3</sub>, Sodium tantalate

1a	It was reported by MATTHIAS in 1949 that NaTaO <sub>3</sub> is ferroelectric below 480 °C. No anomalies of the dielectric constants, however, were observed by SMOLENSKII et al.					49M1 57S3
b	phase	IV	III	II	I	
	state	(F)				
	crystal system	orthorhombic	orthorhombic	tetragonal	cubic	
	space group	Pc <sub>2</sub> n-C <sub>2v</sub>				
	$\Theta$	480	550	630	°C	
	$a = 5.4941 \text{ \AA}$ , $b = 7.7508 \text{ \AA}$ , $c = 5.5130 \text{ \AA}$ at RT. The cubic cell in phase I becomes pseudomonoclinic in phase IV. Relation between the orthorhombic unit cell and the pseudomonoclinic cell: Fig. 21.					2a 57K1 57K1 62I4 51V2
3	Crystal structure: $Z = 4$ . Atomic positions: Tab. 9; Fig. 22.					
4	Temperature dependence of lattice parameters: Tab. 10; Fig. 23.					

Tab. 9.  $\text{NaTaO}_3$ . Fractional coordinates of atoms in the unit cell.  
[57K1]

Na	$x: 0 - 0.01$	$0 + 0.01$	$\frac{1}{2} - 0.01$	$\frac{1}{2} + 0.01$
	$y: \frac{1}{4} + 0.03$	$\frac{1}{4} + 0.03$	$\frac{1}{4} + 0.03$	$\frac{1}{4} + 0.03$
	$z: 0 + 0.02$	$0 - 0.02$	$\frac{1}{2} - 0.02$	$\frac{1}{2} + 0.02$
Ta*	$x: \frac{1}{2}$	$\frac{1}{2}$	0	0
	$y: 0$	$\frac{1}{2}$	$\frac{1}{2}$	0
	$z: 0$	0	$\frac{1}{2}$	$\frac{1}{2}$
O(1)	$x: 0 - 0.02$	$0 + 0.02$	$\frac{1}{2} + 0.02$	$\frac{1}{2} - 0.02$
	$y: \frac{1}{4} + 0.01$	$\frac{1}{4} + 0.01$	$\frac{1}{4} + 0.01$	$\frac{1}{4} + 0.01$
	$z: \frac{1}{2} + 0.02$	$\frac{1}{2} - 0.02$	$0 + 0.02$	$0 - 0.02$
O(2)	$x: \frac{1}{4} + 0.04$	$\frac{1}{4} - 0.04$	$\frac{3}{4} - 0.04$	$\frac{3}{4} + 0.04$
	$y: 0 - 0.03$	$0 - 0.03$	$\frac{1}{2} - 0.03$	$\frac{1}{2} - 0.03$
	$z: \frac{1}{4} + 0.04$	$\frac{1}{4} + 0.04$	$\frac{3}{4} - 0.04$	$\frac{3}{4} - 0.04$
O(3)	$x: \frac{1}{4} + 0.04$	$\frac{1}{4} - 0.04$	$\frac{3}{4} - 0.04$	$\frac{3}{4} + 0.04$
	$y: \frac{1}{2} + 0.06$	$\frac{1}{2} + 0.06$	$0 + 0.06$	$0 + 0.06$
	$z: \frac{1}{4} + 0.04$	$\frac{1}{4} + 0.04$	$\frac{3}{4} - 0.04$	$\frac{3}{4} - 0.04$

Tab. 10.  $\text{NaTaO}_3$ . Temperature dependence of the pseudo-cell parameters. [62I4].  
For the notations, see Fig. 21

$T$ [°C]	23	100	200	300	400	450	480	500	550	580	600
$a' = c' [\text{\AA}]$	3.889 <sub>s</sub>	3.893 <sub>s</sub>	3.899 <sub>s</sub>	3.907	3.912 <sub>s</sub>	3.916	3.918	3.920	3.923	3.925 <sub>s</sub>	3.927
$b' [\text{\AA}]$	3.885 <sub>s</sub>	3.890 <sub>s</sub>	3.896 <sub>s</sub>	3.903 <sub>s</sub>	3.910 <sub>s</sub>	3.913 <sub>s</sub>	3.915 <sub>s</sub>	3.918	3.923	$\approx 3.925_s$	$\approx 3.927$
$\beta - 90^\circ$	22'00"	16'00"	9'00"	6'00"	4'00"	3'30"	2'00"	$\approx 2'00"$	1'30"	0'00"	0'00"
$a'/b'$	1.0010	1.0009	1.0009	1.0008	1.0006	1.0006	1.0005	1.0005	1.000	1.000	1.000
$V$ [ $\text{\AA}^3$ ]	58.8 <sub>s</sub>	59.0 <sub>s</sub>	59.2 <sub>s</sub>	59.5 <sub>s</sub>	59.8 <sub>s</sub>	60.0 <sub>s</sub>	60.1 <sub>s</sub>	60.2 <sub>s</sub>	60.3 <sub>s</sub>	60.4 <sub>s</sub>	60.5 <sub>s</sub>
	$T$ [°C]	630	660	680							
	$b = a = c$ [ $\text{\AA}$ ]	3.929	3.931	3.932 <sub>s</sub>							
	$V$ [ $\text{\AA}^3$ ]	60.6 <sub>s</sub>	60.7 <sub>s</sub>	60.8 <sub>s</sub>							

Nr. 1A-4  $\text{KTaO}_3$ , Potassium tantalate

1a	Ferroelectric activity was first reported by MATTHIAS in 1949; <sup>a)</sup> however, recent studies by WEMPLE have proved that the ferroelectric transition does not occur, at least above 1.6 °K. <sup>b)</sup>	<sup>a) 49M1, 49M4</sup> <sup>b) 64W2, 65W2</sup>
b	$\text{KTaO}_3$ is cubic and its space group is $\text{Pm}3\text{m-O}_h$ . $T_{\text{met}} = (1357 \pm 3)$ °C. $\rho = 6.97 \cdot 10^3 \text{ kg m}^{-3}$ . $a = 3.9885 \text{ \AA}$ at RT. Transparent, colorless or pale blue (blue in oxygen-deficient crystals). Cleavage: along (100) planes. Hardness: nearly the same as quartz.	<sup>64W2, 65W2, 51V2 55R2, 56R2 58R1 51V2 64W2</sup>
2a	Flux method: KF flux, <sup>a)</sup> dark small crystals; $\text{K}_2\text{CO}_3$ flux, <sup>b)</sup> large ( $\approx 10$ mm) transparent crystals. Czochralski-Kyropoulos method: large ( $\approx 10$ mm) good quality crystals. Floating technique: planar single crystals. Phase diagram of system $\text{K}_2\text{CO}_3\text{-Ta}_2\text{O}_5$ : Fig. 24. Hydrothermal phase diagram $\text{K}_2\text{O}\text{-Ta}_2\text{O}_5\text{-H}_2\text{O}$ at 400 °C:	<sup>a) 62T5, 64W2 b) 66U1 64W2, 65W2, 67B7 66W8</sup> 67M2
3	$Z = 1$ Crystal structure: cubic perovskite type, ( $\text{Pm}3\text{m-O}_h$ ). K at 1a position; Ta at 1b position; O at 3c position.	<sup>51V1, 51V2</sup>

\* All positions  $\pm 0.002$ .

## II 1 Oxide des Perowskit-Typs

Figuren S. 221ff.

<p>4 Nr. 1A-4 <math>\text{KTaO}_3</math> continued  <math>a = 3.9885 \text{ \AA}</math> at RT; <math>a = 4.0026 \text{ \AA}</math> at <math>450^\circ\text{C}</math>.</p> <p>5a Dielectric constant at low frequencies: earlier studies showed a peak in the <math>\kappa</math> vs. <math>T</math> curve;<sup>a)</sup> recent measurements have shown that no peak exists down to <math>1.6^\circ\text{K}</math>.<sup>b)</sup> Fig. 25.  <math>\kappa = 243</math> at RT.  <math>\kappa = \kappa_0 + C/(T - \Theta_p)</math> <math>T &gt; 30^\circ\text{K}</math>, where <math>\kappa_0 = 48</math>, <math>C = 5.7 \cdot 10^4 \text{ }^\circ\text{K}</math>, <math>\Theta_p = 4^\circ\text{K}</math>.  Loss tangent: <math>\tan \delta \approx 0.001</math> at <math>200 \text{ kHz}</math> at RT.  Dielectric constant in the GHz range: Fig. 26.  <math>Q</math> values in the GHz range: <math>Q = 10^3 \dots 10^4</math>.  Dielectric loss in the far infrared frequency range: See 1A-4-9 below (Figs. 34, 35).  Hydrostatic pressure dependence of the reciprocal dielectric constant: Fig. 27.</p> <p>b Effects of dc bias on <math>\kappa</math> at <math>4.2^\circ\text{K}</math> and at RT: Figs. 28, 29.  Coefficients in free energy expansion:  <math>\xi = 9 \cdot 10^9 \text{ V m}^5 \text{ C}^{-3}</math> at <math>4.2^\circ\text{K}</math>, <math>\xi = (4 \pm 1) \cdot 10^9 \text{ V m}^5 \text{ C}^{-3}</math> at <math>295^\circ\text{K}</math>.</p> <p>c <math>D</math> vs. <math>E</math> curves show no hysteresis character down to <math>1.6^\circ\text{K}</math>.  <math>P</math> vs. <math>E</math> at <math>4.2^\circ\text{K}</math>: see</p>	<p>51V2, 59B1</p> <p><sup>a)</sup>50H3  <sup>b)</sup>65W2, 64W2  65W2  64W2  64R3  64W2  65K1  65W2  64W2</p>	<p>12a  b  13b</p>
<p>9a Refractive index in visible region: Fig. 30.  Reflectivity in far infrared region and the dispersion: Figs. 31, 32.  Reflectivity data were used to obtain transverse optical modes of the lattice vibration by means of Kramers-Kronig relation (cf. Tab. 42).  Transverse optical modes as a function of temperature: Tab. 11; Fig. 33.  The square of the wave number <math>\tilde{\nu}_{11}</math> for the "ferroelectric mode" is approximately linear to <math>T</math>: <math>\tilde{\nu}_{11}^2 \propto (T - \Theta_p)</math>.  (Additional data are given on the ferroelectric soft mode, see 1A-4-13b).  Effect of lattice vibration on the fluorescent spectrum of <math>\text{Eu}^{3+}</math> in <math>\text{KTaO}_3</math>; see  Imaginary part of the dielectric constant and the conductivity in the far infrared region: Figs. 34, 35.  Absorption coefficient <math>\alpha</math> depends on the degree of oxygen reduction in <math>\text{KTaO}_3</math>.  Absorption coefficient near the interband absorption edge (about 3.6 eV) for insulating and semiconducting <math>\text{KTaO}_3</math>; Fig. 36 (for additional data, see Fig. 2 of reference).  Absorption vs. wavelength of light: Fig. 37.  Absorption vs. carrier concentration in semiconducting <math>\text{KTaO}_3</math>: Fig. 38.  Optical absorption in impurity doped single crystals: for impurities Fe, Mn, Co and Cr, see</p> <p>b Quadratic electrooptic constants (<math>6328 \text{ \AA}</math>, <math>2 \dots 77^\circ\text{K}</math>):  <math>M_{11} - M_{12} = (0.16 \pm 0.01) \text{ m}^4 \text{ C}^{-2}</math>; <math>M_{44} = (0.12 \pm 0.01) \text{ m}^4 \text{ C}^{-2}</math>.  Electroreflectance and electroabsorption were studied using semiconducting <math>\text{KTaO}_3</math>.  Effect of interface dc field on the reflectance of the (100) surface: Fig. 39.  Electroreflectance spectra of (100) and (111) surfaces: Figs. 40, 41.  Electroreflectance spectra of (100) and (111) surfaces: Figs. 40, 41.  Effect of polarization of light on the electroreflectance: Fig. 42.  Electroreflectance as a function of the surface polarization: Fig. 43.  Electroreflectance singularities and the corresponding energies: Tab. 12.  Electroabsorption near the absorption edge: Fig. 44.  Fundamental absorption edge (<math>\approx 3.6 \text{ eV}</math>) shifts to higher energies with dc bias: Fig. 45.</p> <p>d Faraday rotation near the band edge: Fig. 46; Tab. 44.</p> <p>f Electric-field-induced Raman effect: Fig. 47.  (For the ferroelectric soft mode obtained from the Raman scattering, see Fig. 33).  Fluorescence spectrum of <math>\text{Eu}^{3+}</math> in <math>\text{KTaO}_3</math>; see</p>	<p>63M4, 67P4  67P4, 67F2  65S9  65W2  67B1  64W2  64G3, 63G3  67F4  67B1, 66B2  67F2  65S9  65W2  65W2</p>	<p>17  Tab.  mode  The  soft  1:  12:  23:  29:  46:  T [<math>^\circ</math>]</p>
<p>10 Resistivity of insulating single crystal: <math>\rho &gt; 10^8 \Omega \text{m}</math> at RT.  Most data on the transport properties have been obtained using oxygen-deficient semiconducting <math>\text{KTaO}_3</math>.  Resistivity of oxygen-deficient single crystals as a function of temperature: Fig. 48.  Hall mobility: <math>\mu_H = 3 \cdot 10^{-8} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}</math> at RT (see also Tab. 13).  <math>\mu_H \approx 8 \cdot 10^{-8} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}</math>, <math>T &gt; 100^\circ\text{K}</math>; Fig. 49.  Hall coefficient and Hall mobility at <math>4.2^\circ\text{K}</math> and RT for several semiconducting <math>\text{KTaO}_3</math>; Tab. 13.  Hall mobility vs. carrier concentration: Fig. 50.  Scattering cross section vs. carrier concentration: see  Ca concentration in doped <math>\text{KTaO}_3</math> vs. net ionized donor concentration: see  Electrical conductivity vs. hydrostatic pressure: Fig. 51.  Conductivity in the far infrared region: see Fig. 35.  Seebeck coefficient: <math>Q = 550 \mu\text{V }^\circ\text{K}^{-1}</math> at RT. (Oxygen-deficient <math>\text{KTaO}_3</math> with <math>N = 3.5 \cdot 10^{23} \text{ m}^{-3}</math>).  Effective mass estimated from the Seebeck coefficient: <math>m^* = (0.8 \pm 0.28) m_0</math>.  Photoconductivity vs. <math>h\nu</math> shows a peak at <math>h\nu = 3.58 \text{ eV}</math>.</p>	<p>65W2  65W2  66S17  66W5  65W2  65W2  65W2  65W2</p>	

Sawaguchi

31	12a	NMR of $^{181}\text{Ta}$ in $\text{KTaO}_3$ : spin-lattice relaxation time, $T_1 \approx 10^{-3}$ sec at RT; spin-spin relaxation time, $T_2 \approx 10^{-5}$ sec at RT; nuclear magnetic moment of $^{181}\text{Ta}$ ( $I = 7/2$ ): $p_n = (2.340 \pm 0.001) \mu_n$ (uncorrected); $(p_n = (2.35 \pm 0.01) \mu_n$ , after estimated corrections). Nuclear magnetic acoustic resonance: the absorption data were given for $\Delta m = \pm 2$ transition of $^{181}\text{Ta}$ as a function of the angle between magnetic field and sound axis [100].	60B2															
W2	b	ESR of $\text{Eu}^{2+}$ and $\text{Gd}^{3+}$ in $\text{KTaO}_3$ : Tab. 14. ESR of $\text{Fe}^{3+}$ : $g = 1.99 \pm 0.01$ ; $ a  = (345 \pm 10) \cdot 10^{-2} \text{ m}^{-1}$ at $4.2^\circ\text{K}$ ; $a = (288 \pm 5) \cdot 10^{-2} \text{ m}^{-1}$ at RT ( $\text{Fe}^{3+}$ is on the $\text{Ta}^{3+}$ site). $a = (30 \pm 1) \cdot 10^{-2} \text{ m}^{-1}$ at RT ( $\text{Fe}^{3+}$ is on the $\text{K}^{1+}$ site). ESR Stark effect for $\text{Fe}^{3+}$ : $E_{\text{bias}}$ along [100] induces axial splitting term $D$ ( $D = 12 \cdot 10^{-2} \text{ m}^{-1}$ at $E_{\text{bias}} = 1.0 \text{ MV m}^{-1}$ at $4.2^\circ\text{K}$ ; $D \propto E_{\text{bias}}^2$ ). ESR of $\text{Ni}^{3+}$ located on $\text{Ta}^{3+}$ site (low spin state) and on $\text{K}^{1+}$ site: see ESR in Mn-doped, Co-doped and Cr-doped $\text{KTaO}_3$ : see	67M4 66U1 64W2 67H3 67H3 63W5, 64W2 67H3, 65H2 64W2															
57P4	13b	Phonon dispersion relation for the transverse optical branch: Fig. 52; Tab. 15. Temperature dependence of the ferroelectric soft mode: Fig. 53. The square of the phonon energy of the ferroelectric soft mode can be approximated by $(h\nu)^2 = 10^4 A/\epsilon$ , $40^\circ\text{K} < T < 295^\circ\text{K}$ ; where $A = 2.825$ (meV) $^2$ , $\epsilon(T)$ is the dielectric constant. For the ferroelectric soft mode, see also 1A-4-9a. Phonon energies of the acoustic modes: Fig. 54.	67S11 67S11															
57F2	17	Etchant: single crystal is slowly etched by dilute HF. Band structure and the related properties: see references; also 1A-4-9a, 9b, 9d, 10, and Tab. 12. Band gap energies determined by various methods:	64W2 67F4, 67B1															
63G3		<table border="1"> <thead> <tr> <th>Method</th> <th>296 °K</th> <th>77 °K</th> </tr> </thead> <tbody> <tr> <td>Faraday rotation</td> <td>3.77 eV 3.62 eV</td> <td>3.79 eV 3.65 eV</td> </tr> <tr> <td>Electroreflectance singularities</td> <td>3.57 eV 3.80 eV</td> <td></td> </tr> <tr> <td>Absorption data</td> <td>3.75 eV</td> <td></td> </tr> <tr> <td>Energy at which <math>\alpha \approx 10^6 \text{ m}^{-1}</math></td> <td>3.79 eV</td> <td></td> </tr> </tbody> </table> <p>Cyclotron resonance of semiconducting <math>\text{KTaO}_3</math> at 70 GHz and <math>1.4^\circ\text{K}</math>: microwave skin depth, about <math>30 \mu\text{m}</math>; see reference paper for the microwave absorption vs. magnetic field curves.</p>	Method	296 °K	77 °K	Faraday rotation	3.77 eV 3.62 eV	3.79 eV 3.65 eV	Electroreflectance singularities	3.57 eV 3.80 eV		Absorption data	3.75 eV		Energy at which $\alpha \approx 10^6 \text{ m}^{-1}$	3.79 eV		67B1 65S13
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Tab. 11.  $\text{KTaO}_3$ . Transverse optical modes at various temperatures [67P4]. The wave number  $\tilde{\nu}_{t1}$  (ferroelectric soft mode) is temperature dependent.

$T [\text{°K}]$	$\tilde{\nu}_{t1}$	$\tilde{\nu}_{t2}$	$\tilde{\nu}_{t3}$
	$\cdot 10^2 \text{ m}^{-1}$		
12	25	196	—
126	58	198	551
232	79	198	551
295	88	199	550
463	106	199	—

Tab. 12.  $\text{KTaO}_3$  (Ca-doped). Singularities observed in electroreflectance spectra (in eV) [67F4]. See Figs. 40, 41

	$E_1$	$E_2$	$A_1$	$A'_1$	$A_2$
	[eV]				
$\text{KTaO}_3$ (100)	3.57	3.80	4.40	4.88	5.50
$\text{KTaO}_3$ (111)	—	3.77	4.45	4.90	5.47
$\text{KTaO}_3$ (110)	3.55	3.80	4.47	4.85	5.50

Tab. 13.  $\text{KTaO}_3$  (reduced). Hall coefficient  $R_H$  and Hall mobility  $\mu_H$  at  $295^\circ\text{K}$  and  $4.2^\circ\text{K}$  for single crystals [65W2]. Carrier concentrations  $N$  are calculated from the  $4.2^\circ\text{K}$  Hall coefficient using  $R_H = -1/N_e$

Sample Nr.	$N_{\text{calc}}$ $\text{m}^{-3}$	$R_H$ $\text{m}^3 \text{C}^{-1}$		$\mu_H$ $\text{m}^2 \text{V}^{-1} \text{sec}^{-1}$	
		(295°K)	(4.2°K)	(295°K)	(4.2°K)
1	$3.5 \cdot 10^{23}$	$20.3 \cdot 10^{-6}$	$18 \cdot 10^{-6}$	$2.7 \cdot 10^{-3}$	2.3
2	$6.0 \cdot 10^{23}$	$12.9 \cdot 10^{-6}$	$10.4 \cdot 10^{-6}$	$2.9 \cdot 10^{-3}$	1.9
3	$6.6 \cdot 10^{23}$	$11.5 \cdot 10^{-6}$	$9.4 \cdot 10^{-6}$	$3.1 \cdot 10^{-3}$	1.9
4	$2.4 \cdot 10^{24}$	$3.0 \cdot 10^{-6}$	$2.6 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	1.1
5	$7.8 \cdot 10^{24}$	$1.0 \cdot 10^{-6}$	$0.80 \cdot 10^{-6}$	$3.0 \cdot 10^{-3}$	0.53
6	$1.3 \cdot 10^{25}$	$0.62 \cdot 10^{-6}$	$0.48 \cdot 10^{-6}$	$3.1 \cdot 10^{-3}$	0.34

Tab. 14.  $\text{KTaO}_3$ . Parameters of ESR spectrum of  $\text{Eu}^{2+}$  and  $\text{Gd}^{3+}$  ions, doped in single crystals of  $\text{KTaO}_3$  [66U1]

Para-magnetic center	Site	S	$\mathcal{H}$	$\nu$ GHz	$T$ °K	g-factor	FS		HFS	
							$b_{40}, b_{60}$ $10^{-2} \text{ m}^{-1}$	I	$A$ $10^{-2} \text{ m}^{-1}$	
$\text{Eu}^{2+}$	K <sup>+</sup>	7/2	(8)	9.1	77	$1.990 \pm 0.002$	$b_{40} = (\pm) 16 \pm 2$ $b_{60} = (\pm) 1.2 \pm 0.6$	5/2	$ ^{151}\text{A}  = 36 \pm 1$	
					4.2	$1.990 \pm 0.002$	$b_{40} = -8.14 \pm 0.27$ $b_{60} = +0.47 \pm 0.3$	5/2	$ ^{153}\text{A}  = 16 \pm 1$	
		7/2			77	$1.990 \pm 0.002$	$b_{40} = -7.0 \pm 0.3$ $b_{60} = +0.5 \pm 0.5$			

Nr. 1A-5  $\text{CaTiO}_3$ , Calcium titanate (Perovskite)

Tab. 16.  $\text{CaTiO}_3$ . Ion positions. [57K2]

4 Ti in 4(a):	$\frac{1}{2}, 0, 0; 0, 0, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 0; 0, \frac{1}{2}, \frac{1}{2}$ .
4 Ca in 4(c):	$x, \frac{1}{2}, z; \bar{x}, \frac{1}{2}, \bar{z}; \frac{1}{2} + x, \frac{1}{2}, \frac{1}{2} - z; \frac{1}{2} - x, \frac{1}{2}, \frac{1}{2} + z;$ with $x = 0, z = 0.030$ .
4 O in 4(c):	with $x = \frac{1}{2} - 0.037, z = -0.018$ .
8 O in 8(d):	$x, y, z; \frac{1}{2} - x, \frac{1}{2} - y, \frac{1}{2} + z;$ $\bar{x}, \frac{1}{2} + y, \bar{z}; \frac{1}{2} + x, \bar{y}, \frac{1}{2} - z;$ $\bar{x}, \bar{y}, \bar{z}; \frac{1}{2} + x, \frac{1}{2} + y, \frac{1}{2} - z;$ $x, \frac{1}{2} - y, z; \frac{1}{2} - x, y, \frac{1}{2} + z;$ with $x = \frac{1}{2} - 0.018, y = -0.026, z = \frac{1}{2} - 0.018$ .

Tab. 15.  $\text{KTaO}_3$ . Phonon energies of the soft ferroelectric mode (transverse optical mode) at various temperatures [67S11]. The wave vector  $q$  at the zone boundary is  $0.788 \text{ \AA}^{-1}$  ( $= \pi/a$ ). See Fig. 52

$T$ °K	Phonon energy [meV] for $q [\text{\AA}^{-1}] =$		
	0	0.1	0.2
295	10.7	11.5	13.5
230	9.7		
170	8.6	10.0	12.5
120	7.3		
77	5.7	7.5	10.7
40	4.2	6.0	
28	3.6	5.9	10.5
15	3.0	5.3	
10	3.2	5.2	
4	3.1	5.3	9.8

1a	Specific heat anomaly associated with a phase transition was observed in $\text{CaTiO}_3$ at about 1260 °C by NAYLOR et al. in 1946. GRÄNICHER et al. reported that $\text{CaTiO}_3$ becomes cubic above 1260 °C.	46N1, 54G1															
b	<table border="1"> <tr> <td>phase</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td></td> <td>P</td> </tr> <tr> <td>crystal system</td> <td>orthorhombic</td> <td>cubic</td> </tr> <tr> <td>space group</td> <td>Pcmn-D<sub>4h</sub><sup>16</sup></td> <td></td> </tr> <tr> <td><math>\Theta</math></td> <td colspan="2"><math>\approx 1260 \text{ }^{\circ}\text{C}</math></td> </tr> </table> <p><math>\rho = 4.10 \cdot 10^3 \text{ kg m}^{-3}</math> at RT.  <math>T_{\text{melt}} = 1960 \text{ }^{\circ}\text{C}</math>  <math>a = 5.3670 \text{ \AA}, b = 7.6438 \text{ \AA}, c = 5.4439 \text{ \AA}</math> at RT.  The ideal perovskite cubic unit cell becomes pseudo-monoclinic in phase II in the same manner as shown in Fig. 21. <math>\beta' = 90^\circ 48'</math> at RT.  Transparent, colorless.</p>	phase	II	I	state		P	crystal system	orthorhombic	cubic	space group	Pcmn-D <sub>4h</sub> <sup>16</sup>		$\Theta$	$\approx 1260 \text{ }^{\circ}\text{C}$		54G1 57K2 46N1 62M3 62M3 57K2
phase	II	I															
state		P															
crystal system	orthorhombic	cubic															
space group	Pcmn-D <sub>4h</sub> <sup>16</sup>																
$\Theta$	$\approx 1260 \text{ }^{\circ}\text{C}$																
2	Flux method; flux: $\text{CaCl}_2, \text{BaCl}_2, \text{CaCl}_2 + \text{BaCl}_2, \text{Na}_2\text{CO}_3 + \text{K}_2\text{CO}_3$ . Flame fusion method:	57K2 58L1, 62M3															
3	Crystal structure: $Z = 4$ in phase II. Fig. 55; Tab. 16.	57K2															
4	Lattice distortion: Fig. 56.	62M3															
5a	Dielectric constant: $\kappa = 186$ , $\tan \delta = 3 \cdot 10^{-4}$ at RT. Fig. 57.																
6a	Specific heat: Fig. 58. Transition heat: $\Delta Q = 550 \text{ cal mol}^{-1}$ at $\Theta_{\text{II}-\text{I}}$ .	46N1															

9a	Nr. 1A-5 CaTiO <sub>3</sub> , continued Refractive indices: Fig. 59. Reflection and absorption: Fig. 60, 61.																
17	Hardness: Mohs 6.5 ... 7, Knoop 986	62M3															
<b>Nr. 1A-6 SrTiO<sub>3</sub>, Strontium titanate</b>																	
1a	Ferroelectric-like behavior of SrTiO <sub>3</sub> was first observed by GRÄNICHER in 1956.	56G2															
b	<table border="1" style="width: 100%; border-collapse: collapse;"> <thead> <tr> <th style="text-align: left;">phase</th> <th style="text-align: center;">II*</th> <th style="text-align: center;">I</th> </tr> </thead> <tbody> <tr> <td>state</td> <td style="text-align: center;">(F)</td> <td style="text-align: center;">P</td> </tr> <tr> <td>crystal system</td> <td style="text-align: center;">tetragonal</td> <td style="text-align: center;">cubic**</td> </tr> <tr> <td>space group</td> <td></td> <td style="text-align: center;">Pm3m-O<sub>h</sub><sup>1</sup></td> </tr> <tr> <td><math>\Theta</math></td> <td style="text-align: center;">110</td> <td style="text-align: center;">°K</td> </tr> </tbody> </table> <p><math>T_{\text{melt}} \approx 2000</math> °C.  <math>\rho = 5.11 \cdot 10^3</math> kg m<sup>-3</sup>.  <math>a = 3.905</math> Å at RT.  Transparent, colorless</p>	phase	II*	I	state	(F)	P	crystal system	tetragonal	cubic**	space group		Pm3m-O <sub>h</sub> <sup>1</sup>	$\Theta$	110	°K	62R1
phase	II*	I															
state	(F)	P															
crystal system	tetragonal	cubic**															
space group		Pm3m-O <sub>h</sub> <sup>1</sup>															
$\Theta$	110	°K															
2a	Crystal growth: Flux method (flux: KF or 50% Na <sub>2</sub> CO <sub>3</sub> + 50% K <sub>2</sub> CO <sub>3</sub> ). Flame-fusion (Verneuil) method. Phase diagram of the system SrO-TiO <sub>3</sub> is given in Figs. 297 and 289 of [64I1].	57N1 61G1 64I1															
3	Crystal structure: $Z = 1$ . Fig. 62.																
4	Thermal expansion: Fig. 63.																
5a	Dielectric constant: Figs. 64 ... 76. Expression of $\kappa$ vs. $T$ curve: Curie-Weiss law: $\kappa = C/(T - \Theta_p)$ , $T > 70$ °K, where $C = 7.83 \cdot 10^4$ °K, $\Theta_p = 28$ °K $\kappa = M/[(T_1/2) \coth(T_1/2 T) - T_0]$ , $T < 50$ °K, where $T_0 = 38$ °K, $T_1 = 84$ °K, $M = 9 \cdot 10^4$ °K.	61M3 59W2, 62S2															
b	Coefficients of free energy expansion at low temperatures:	66C6															
c	Saturation polarization: Fig. 77. Remanent polarization: Fig. 78.																
d	Electrocaloric effect: Fig. 79. For additional data, see	64K5, 65H4, 61H1															
6a	Specific heat: Fig. 80. Specific heat below 1 °K, see	61g1, 66A4															
b	Thermal conductivity: Figs. 81, 82. For ceramics: see also	58Y1, 60Y1, 61g1, 66H9															
7a	Piezoelectricity (dc bias induced piezoelectricity): Figs. 83, 84, 85.																
b	Electrostriction: Fig. 86.																
8a	Elastic compliances and stiffnesses: Tab. 17; Figs. 87, 88, 89.																
9a	Refractive indices: Tabs. 18, 19; Fig. 90. Reflectivity, absorption coefficient and dielectric constant: (i) Infrared region: Figs. 91 ... 95. See also Tab. 42. (ii) Visible and ultraviolet region: Figs. 96 ... 102. See also Tab. 43.																
b.	Quadratic electrooptic effect: $M_{11} - M_{12} = (0.14 \pm 0.01) \text{ m}^4 \text{ C}^{-2}$ at 6328 Å (4.2 ... 300 °K).	64G3															
c	Piezo optic effect: Tabs. 20, 21.																

\* In phase II a hysteresis loop is observed, a), b) but the remanent polarization depends upon the amplitude of the applied field. According to LYTLE, phase II consists of three phases. a) [59W2], b) [61M3], [64L4]

\*\* Generally the phase I is believed to be cubic but evidence of pseudo-cubic structure was reported by a few authors. [64L4], [66C6]

## Figuren S. 236 ff.

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9d	Nr. 1A-6 SrTiO <sub>3</sub> , continued Faraday rotation: Fig. 103. See also Tab. 44.	67B1
e	Raman effect: Fig. 104. Brillouin scattering: Fig. 105. See	66K1 61g1 61g1
10	Electrical resistivity: $\rho > 10^7 \Omega\text{m}$ (good quality single crystal) at RT. Fig. 106. For additional data, see Tab. 22. Resistivity, Hall coefficient and Hall mobility of semiconductive samples: Tab. 23; Figs. 107 ... 110. For additional data, see Hall mobility for photo-excited electron: see Fig. 115. Piezoresistivity: Figs. 111, 112, 113. Photoconductivity: Figs. 114, 115. Photoemission: Fig. 116. Superconductivity: discovered in semiconductive SrTiO <sub>3</sub> by SCHOOLEY et al. in 1964. Figs. 117 ... 120. Tab. 24. Penetration depth of static magnetic field in superconductive SrTiO <sub>3</sub> is of the order of $10^{-5} \text{ m}$ .	64F5, 67T6 66T10 64S5 66S16
11	Magnetic susceptibility: Tab. 25.	
12a	NMR: Fig. 121.	
b	ESR: Tab. 26; Figs. 122 ... 130.	
c	Mössbauer effect: Figs. 131, 132.	
13c	Inelastic neutron scattering: Tab. 27; Figs. 133, 134, 135.	
14a	Domain structure: A fine twin structure was observed in phase II. The appearance of the twin structure is similar to that of the 90° domains in tetragonal BaTiO <sub>3</sub> . The dc field, however, does not change the twin structure.	61M3, 64L4
16	Radiation damage: Fig. 136.	
17	Etching and chemical polishing: Band structure and related properties: The band structure was determined theoreti- cally by KAHN et al.: Fig. 137. For discussions, see Magnetoresistance, Shubnikov-deHaas effect. The conduction band consists of spheroids along [100] having 3 minima at $X_s$ . The $m_t = 1.5 m_0 (\pm 15\%)$ , $m_1 = 6.0 m_0 (\pm 30\%)$ .	66R6 64K1 65S18 66F3, 67F3 67F3

Tab. 17. SrTiO<sub>3</sub>. Elastic constants at RT

$s_{11}$	$s_{12}$	$s_{13}$	$c_{11}$	$c_{12}$	$c_{13}$	Method	Note	Reference
$10^{-12} \text{ m}^2 \text{ N}^{-1}$			$10^{11} \text{ N m}^{-2}$					
3.3	-0.74	8.4	3.48	1.01	1.19	composite- bar pulse	$c$ calculated from $s$	58p5
3.729	-0.909	8.091	3.181	1.025	1.236	composite- bar pulse	$s$ calculated from $c$	63B2
3.772 $\pm 0.023$	-0.926 $\pm 0.010$	8.233 $\pm 0.040$	3.156 $\pm 0.027$	1.027 $\pm 0.027$	1.215 $\pm 0.006$		$s$ calculated from $c$	63W1

Tab. 18. SrTiO<sub>3</sub>.  $n$  vs.  $\lambda$  at 21 °C. [57G1]

$\lambda$ Å	$n$	$\lambda$ Å	$n$	$\lambda$ Å	$n$
4200	2.6050	5400	2.4386	6600	2.3771
4300	2.5810	5500	2.4312	6700	2.3737
4400	2.5585	5600	2.4245	6800	2.3703
4500	2.5394	5700	2.4182	6900	2.3674
4600	2.5236	5800	2.4122	7000	2.3645
4700	2.5101	5900	2.4069	7100	2.3617
4800	2.4970	6000	2.4019	7200	2.3590
4900	2.4846	6100	2.3971	7300	2.3564
5000	2.4734	6200	2.3928	7400	2.3538
5100	2.4636	6300	2.3886	7500	2.3514
5200	2.4548	6400	2.3846	7600	2.3490
5300	2.4464	6500	2.3807	7700	2.3468

Tab. 19. SrTiO<sub>3</sub>.  $n$  vs.  $\lambda$  [65B9]

$\lambda$ μm	$n$	$\lambda$ μm	$n$
0.45	2.537	1.8	2.270
0.5	2.472	2.0	2.264
0.6	2.402	2.2	2.258
0.7	2.363	2.4	2.2524
0.8	2.340	2.6	2.2490
0.9	2.326	2.8	2.2395
1.0	2.315	3.0	2.2315
1.1	2.306	3.2	2.2236
1.2	2.299	3.4	2.2143
1.4	2.287	3.6	2.2058
1.6	2.279	3.8	2.1951

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Tab. 20.  $\text{SrTiO}_3$ .  $\Pi_{66}$  vs.  $\lambda$  at  $(27 \pm 1)^\circ\text{C}$ . [57G1]

$\lambda$ Å	$\Pi_{66}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$	$\lambda$ Å	$\Pi_{66}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$
4200	-3.69	6000	-4.92
4300	-3.74	6100	-4.99
4400	-3.78	6200	-5.05
4500	-3.99	6300	-5.12
4600	-3.965	6400	-5.13
4700	-4.13	6500	-5.18
4800	-4.09	6600	-5.22
4900	-4.22	6700	-5.29
5000	-4.33	6800	-5.52
5100	-4.32	6900	-5.48
5200	-4.41	7000	-5.555
5300	-4.51	7100	-5.62
5400	-4.59	7200	-5.77
5500	-4.575	7300	-5.73
5600	-4.62	7400	-5.78
5700	-4.69	7500	-5.79
5800	-4.79	7600	-5.825
5900	-4.85	7700	-5.98

Tab. 21.  $\text{SrTiO}_3$ .  $\Pi_{21} - \Pi_{11}$  vs.  $\lambda$  at  $(27 \pm 1)^\circ\text{C}$ . [57G1]

$\lambda$ Å	$\Pi_{21} - \Pi_{11}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$	$\lambda$ Å	$\Pi_{21} - \Pi_{11}$ $10^{-13} \text{ m}^2 \text{ N}^{-1}$
4200	9.03	6000	9.95
4300	9.23	6100	9.94
4400	9.03	6200	9.91
4500	9.26	6300	9.84
4600	9.12	6400	9.82
4700	9.12	6500	9.88
4800	9.14	6600	9.96
4900	9.16	6700	9.92
5000	9.35	6800	9.98
5100	9.44	6900	9.99
5200	9.61	7000	9.91
5300	9.54	7100	9.92
5400	9.68	7200	9.94
5500	9.56	7300	9.99
5600	9.85	7400	10.05
5700	9.85	7500	9.90
5800	9.86	7600	9.92
5900	9.88	7700	10.02

Tab. 22.  $\text{SrTiO}_3$  (single crystal). Effects of electrode material on the apparent conductivity [65C6]. Measurements were made by the two terminal method at  $T = 130^\circ\text{C}$ ,  $t = 24$  hours after the application of the field  $E = 100 \text{ kV m}^{-1}$ 

Electrode material	$\sigma [\Omega^{-1} \text{ m}^{-1}]$ after 24 h at $130^\circ\text{C}$	Form of $\sigma$ vs. $t$ curve	
		After 24 h	After 24 h
Au	$4.8 \cdot 10^{-7}$	Fall then rise	
Ag	$8.8 \cdot 10^{-8}$	As for gold	
Sn	$8.8 \cdot 10^{-9}$	Fall followed by slow rise but without saturation	
Cr	$6.0 \cdot 10^{-11}$	Continuous fall tending toward steady value	
Cd	$9.5 \cdot 10^{-11}$	Similar to chromium	
Al	$2.9 \cdot 10^{-10}$	Similar to chromium (for a field of $400 \text{ kV m}^{-1}$ behavior is like that of gold)	

Tab. 23.  $\text{SrTiO}_3$  (single crystal). The  $300^\circ\text{K}$  and  $2^\circ\text{K}$  Hall coefficient  $R_H$  and Hall mobility  $\mu_H$  values and the  $300^\circ\text{K}$  electron concentrations for semiconductive single crystals. [67T6]. In the first column, (Nb) means Nb-doped samples, the other samples are reduced ones

Sample	300 °K		2 °K		$n = \frac{1}{eR_H (300^\circ\text{K})}$ $\text{m}^{-3}$
	$R_H$ $10^{-6} \text{ m}^3 \text{ C}^{-1}$	$\mu_H$ $10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$	$R_H$ $10^{-6} \text{ m}^3 \text{ C}^{-1}$	$\mu_H$ $10^{-1} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$	
5	0.26	6.5	0.25	1.0	$2.4 \cdot 10^{25}$
2	0.62	5.2	0.77	1.8	$1.0 \cdot 10^{25}$
3	1.8	7.2	3.9	2.7	$3.5 \cdot 10^{24}$
6	5.3	8.0	11.0	3.1	$1.2 \cdot 10^{24}$
12	14.0	8.0			$4.5 \cdot 10^{23}$
9	23.0	5.8			$2.7 \cdot 10^{23}$
13(Nb)	0.22	5.5	0.22	3.3	$2.8 \cdot 10^{25}$
8(Nb)	0.58	4.8	0.63	8.2	$1.1 \cdot 10^{25}$
10(Nb)	3.4	6.2	3.3	12.0	$1.8 \cdot 10^{24}$
14(Nb)	14.0	6.7	11.0	13.0	$4.5 \cdot 10^{23}$
15(Nb)	22.0	5.4	18.0	19.0	$2.8 \cdot 10^{23}$
11(Nb)	44.0	6.0	33.0	22.0	$1.4 \cdot 10^{23}$

Tab. 24 see page 50

Tab. 25.  $\text{SrTiO}_3$ . Susceptibility in pure and reduced single crystals [66F2].  
 $\Delta\chi_{\text{magn}}$  represents the contribution from the charge carriers;  $\Delta\chi_{\text{magn}}^*$  is obtained by measuring the  
 $\chi_{\text{magn}}$  of reduced crystals and subtracting the "pure" diamagnetic and Van Vleck contributions.  
 $N$  = carrier concentration;  $T_{\text{deg}}$  = degeneracy temperature;  $m^*$  = density-of-state effective mass

Sample	$N$ at 4.2 °K $\text{m}^{-3}$	$T_{\text{deg}}$ °K	$\chi_{\text{magn}}$ or $\Delta\chi_{\text{magn}} \cdot 10^{-7} \text{ cm}^3 \text{ g}^{-1}$	78 °K	4.2 °K	$m^*$ at 4.2 °K [ $\text{m}_0$ ]
Pure						
28 h, 950 °C hydrogen	$6 \cdot 10^{24}$	28	$\chi$	-1.02 +0.037 +0.270	-1.00 +0.073 +0.523	-0.92 -0.928 5.1
5 h, 1200 °C hydrogen (carbon boat)	$7.5 \cdot 10^{25}$	148	$\frac{\Delta\chi_1}{\Delta\chi_3}$			
reoxidized 18 h, 700 °C, air	-	-	$\chi$	-1.016	-1.012	-0.919
27 h, 1370 °C hydrogen (carbon boat)	$5.3 \cdot 10^{26}$	550	$\Delta\chi_3$	+1.704	+1.763	-
						4.9

<sup>a)</sup> [62B2]    <sup>b)</sup> [62S12]

Tab. 27.  $\text{SrTiO}_3$ . The frequency of the lowest transverse optic mode at  $q = 0$  for five different temperatures. [62C4]

Sample	$N$ at 4.2 °K $\text{m}^{-3}$	$T_{\text{deg}}$ °K	$\chi_{\text{magn}}$ or $\Delta\chi_{\text{magn}} \cdot 10^{-7} \text{ cm}^3 \text{ g}^{-1}$	$10^{18} \text{ sec}^{-1}$		$T$ °K	$10^{18} \text{ sec}^{-1}$
				300 °K	78 °K	4.2 °K	Neutron
Pure							
28 h, 950 °C hydrogen	$6 \cdot 10^{24}$	28	$\chi$	-1.02 +0.037 +0.270	-1.00 +0.073 +0.523	-0.92 -0.928 5.1	90 142 203 296
5 h, 1200 °C hydrogen (carbon boat)	$7.5 \cdot 10^{25}$	148	$\frac{\Delta\chi_1}{\Delta\chi_3}$	$\chi$	-1.016	-1.012	2.24 2.73
reoxidized 18 h, 700 °C, air	-	-				-	0.05 0.05
27 h, 1370 °C hydrogen (carbon boat)	$5.3 \cdot 10^{26}$	550	$\Delta\chi_3$	+1.704	+1.763	-	4.9 3.32 0.07
							3.0 <sup>a)</sup> 2.63 <sup>b)</sup>

<sup>a)</sup> [62B2]    <sup>b)</sup> [62S12]

Tab. 26.  $\text{SrTiO}_3$ . Summary of the properties of ESR spectrum in  $\text{SrTiO}_3$  for various doped paramagnetic ions

Para-magnetic center	Site	S	$\mathcal{H}$	$\nu$ GHz	$T$ °K	$g$ -factor		FS	HFS	Ref.	Literature
						$g_{  }$	$g_{\perp}$				
$\text{Cr}^{3+}$	$\text{Ti}^{4+}$	3/2	(5)	9	80	$1.9788 \pm 0.007$	(isotropic)	$D = 2 \pm 0.3$ , $E = 0$	${}^{19}\mathcal{A} = 0$	3/2	58M7
					300	$1.9780 \pm 0.007$	(isotropic)	$D = 0$ , $E = 0$	${}^{55}\mathcal{A} = 16.2 \pm 0.3$		62M6
$\text{Mn}^{4+}$	$\text{Ti}^{4+}$	3/2	(5)	10	77	$1.994 \pm 0.001$	(isotropic)	$D = +1.0$ , $E = 0$	${}^{55}\mathcal{A} = -69.4 \pm 1$	5/2	59M4
$\text{Fe}^{3+}$	$\text{Ti}^{4+}$	5/2	(7)	9	1.9	$2.004 \pm 0.001$	(isotropic)	$D = -0.7$ , $E = 0$	${}^{55}\mathcal{A} = -69.4 \pm 1$		
					4.2	$2.004 \pm 0.001$	(isotropic)	$D = +17.9 \pm 1.0$ , $E = 0$	${}^{55}\mathcal{A} = -230 \pm 10$	0	59D2
					77	$2.004 \pm 0.001$	(isotropic)	$D = +16.1 \pm 0.7$ , $E = 0$	${}^{55}\mathcal{A} = -225.6 \pm 1.9$		58M8
					300	$2.004 \pm 0.001$	(isotropic)	$D = +7.3 \pm 0.3$ , $E = 0$	${}^{55}\mathcal{A} = -220.8 \pm 1.1$		
$\text{Ni}^{3+}$	$\text{Ti}^{4+}$	1	(4)	10	80	$2.204 \pm 0.001$	(isotropic)	$D = 1.0$ , $E = -197.7 \pm 0.7$			
$\text{Ni}^{1+}$ or $\text{Ni}^{3+}$	$\text{Ti}^{4+}$	1/2	(2)	10	20	$2.029 \pm 0.001$	(isotropic)				
					80						
					203						

Para-magnetic center	Site	S	$\mathcal{H}$	$\nu$ GHz	$T$ °K	$g$ -factor		FS	HFS	Ref.	Literature
						$g_{  }$	$g_{\perp}$				

$\text{Ni}^{2+}$	$\text{Ti}^{4+}$	1	(4)	10	uv	vv
$\text{Ni}^{2+}$ or $\text{Ni}^{3+}$	$\text{Ti}^{4+}$	1/2	(2)	10	20	20
				80	2.029 $\pm$ 0.001	2.352 $\pm$ 0.001
				203		

Para-magnetic center	Site	S	$\mathcal{K}$	GHz	$T$ °K	g-factor			FS		HFS		Ref.	Literature
						$g_{\parallel}$	$g_{\perp}$	$g_{\perp}$	$D, E, \alpha [10^{-4} \text{ m}^{-1}]$	$I$	$\Delta A_{\parallel}, \Delta A_{\perp} [10^{-2} \text{ m}^{-1}]$			
Ni <sup>3+</sup>	Ti <sup>4+</sup>	1/2	(2)	10	4.2	2.110 ± 0.002	2.213 ± 0.002							62R3
				20	2.136 ± 0.001	2.202 ± 0.001								
		203		80	2.172 ± 0.001	2.184 ± 0.001								62R3
					(isotropic)	2.180 ± 0.002								62R3
Ce <sup>3+</sup>	—	1/2	(2)	10	4.2	3.005 ± 0.005	1.118 ± 0.003							f)
Nd <sup>3+</sup>	—	1/2	(2)	10	4.2	2.609 ± 0.003	2.472 ± 0.003							62R2
				16	2	2.61 ± 0.01	2.470 ± 0.005							
		35		35	2	2.62 ± 0.01	2.470 ± 0.005							62R2
				16	2	2.11 ± 0.01	2.780 ± 0.005							
Yb <sup>3+</sup>	—	1/2	(3)	35		2.10 ± 0.005								62R2
				35										
		50		16	50	2.18 ± 0.01	2.720 ± 0.005							
				35		2.17 ± 0.005	2.720 ± 0.005							
Eu <sup>2+</sup>	—	65		35	65	(2.25)	2.70 ± 0.01							62R2
		16	(8)	16	2	1.99 ± 0.001	-10 ± 4	106.6 ± 2		6.7 ± 2				62R2
				300		1.99 ± 0.001	0	105.9 ± 2		1.1 ± 2				
Gd <sup>3+</sup>	Sr <sup>2+</sup>	7/2	(8)	16	2	1.992 ± 0.002	-362.5 ± 0.5	-3.2 ± 0.5		1.4 ± 0.5				62R2
				12, 18	4.2	1.992 ± 0.002	-362.5 ± 0.5	-3.24 ± 0.5		1.4 ± 0.5				62R1
		77		77		1.992 ± 0.002	-233.6 ± 0.5	-4.8 ± 0.5		-0.25 ± 0.5				
				300		1.992 ± 0.002				-5.7 ± 0.2	0.5 ± 0.3			

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- a)  $\xi = [100]$ ,  $\eta = [010]$ ,  $\zeta = [001]$ .  
 b) Deviations from spin Hamiltonian (7) are ascribed to a covalent bonding by MÜLLER. However, AISENBERG et al. find a negligible contribution of the covalent bonding. [59A1].  
 c) Spectrum is due to a double quantum absorption between  $S_z = -1$  and  $S_z = +1$  levels.  
 d) At least fifteen inequivalent sites are observed.  
 e) Three inequivalent spectra are observed with axes parallel to the cubic [100], [010] and [001].  
 f) Effects of temperature and pressure on  $\text{Ca}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Eu}^{2+}$ , and  $\text{Gd}^{3+}$  spectra. [64R2].  
 g)  $\text{Fe}^{2+}$  spectra due to nearest charge compensation. [64K7].  
 h) Directional dependence of  $\text{Gd}^{3+}$  spectrum. [66S1].

Tab. 24.  $\text{SrTiO}_3$  (ceramics containing Ba or Ca in mol%). Superconductive properties of  $(\text{Ba}_x\text{Sr}_{1-x})\text{TiO}_3$  and  $(\text{Ca}_x\text{Sr}_{1-x})\text{TiO}_3$  [67S8].  $H_{c1}$  is the point at which the magnetization curve first deviates from linearity;  $H_{c1}(0)$  is the extrapolated value for  $T \rightarrow 0$  °K.  
 $N$  = Carrier concentration       $\Theta_c$  = superconducting transition temperature

% Ba or Ca	$N$ $10^{25} \text{ m}^{-3}$	$\Theta_c$ °K	$H_{c1}(0)$ Oe	% Ba or Ca	$N$ $10^{25} \text{ m}^{-3}$	$\Theta_c$ °K	$H_{c1}(0)$ Oe
—	2.7	0.18		10.0	4.2	0.25	
—	5.8	0.30	2.8	12.5	4.5	<0.10	
—	6.4	0.25	2.8				
—	1.7	0.10		2.5 (Ca)	5.0	0.32	
—	12.0	0.17		5.0	9.2	0.30	
—	23.0	0.10		7.5	74.0	<0.06	
2.5 (Ba)	6.0	0.52		7.5	8.7	0.43	(3.5) <sup>a)</sup>
2.5	0.3	0.23		7.5	0.2	<0.06	
5.0	6.7	0.50	3.9	7.5	0.6	0.37	
7.5	7.0	0.29		7.5	33.0	<0.07	
7.5	0.05	0.22		7.5	2.0	0.48	
7.5	34.0	0.09		10.0	0.06 <sup>b)</sup>	<0.06	
7.5	0.5	0.25		20.0	9.3	0.39	
7.5	2.3	0.27		30.0	13.0	0.29	
7.5	15.0	0.45		30.0	6.7	0.50	
				30.0	0.6	<0.05	1.9

Nr. 1A-7  $\text{CdTiO}_3$ , Cadmium titanate

1a	$\text{CdTiO}_3$ was reported by SMOLENSKII in 1950 to be ferroelectric below 50 ... 60 °K. In 1950 HULM et al. denied its ferroelectricity but HEGENBARTH supported SMOLENSKII's findings.							50S7, 50H2, 59H4					
b	phase												
	state	II (F) <sup>a)</sup>	I										
	crystal system	orthorhombic <sup>b)</sup>											
	space group	$\text{Pc}2_1\text{n}^b)$ - $\text{C}_{2v}^b$											
	$\Theta$	—223 ... —213 °C Lattice constants: $a = 5.348 \text{ \AA}$ , $b = 7.615 \text{ \AA}$ , $c = 5.417 \text{ \AA}$ at RT. The relation between the orthorhombic unit cell and the pseudo-cubic monoclinic cell is the same as in the case of $\text{NaTaO}_3$ ; see Fig. 21.											
2	Flux method (flux: 40 wt% NaCl + 40 wt% $\text{NaBO}_2$ + 20 wt% $\text{Na}_2\text{CO}_3$ ).							57K1					
3	$Z = 4$ . Crystal structure in phase I: Tab. 28; Fig. 138.												
5a	Dielectric constant: $\kappa = 250$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 4.5 \cdot 10^4 \text{ \textcircled{K}}$ .							50S7, 50H2					
b	Effect of $E_{\text{bias}}$ on $\kappa$ : Fig. 139.												

Tab. 28. $\text{CdTiO}_3$ . Fractional coordinates of atoms in the unit cell. [57K1]	Cd	Positions					Estimated error
		$x$ :	$0 + 0.006$	$0 - 0.006$	$\frac{1}{2} + 0.006$	$\frac{1}{2} - 0.006$	
		$y$ :	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{1}{4}$	$\pm 0.002$
		$z$ :	$0 + 0.016$	$0 - 0.016$	$\frac{1}{2} - 0.016$	$\frac{1}{2} + 0.016$	$\pm 0.002$
	Ti	$x$ :	$\frac{1}{2} + 0.005$	$\frac{1}{2} - 0.005$	$0 + 0.005$	$0 - 0.005$	$\pm 0.005$
		$y$ :	0	$\frac{1}{2}$	$\frac{1}{2}$	0	$\pm 0.005$
		$z$ :	$0 - 0.065$	$0 + 0.065$	$\frac{1}{2} + 0.065$	$\frac{1}{2} - 0.065$	$\pm 0.010$
	O(1)	$x$ :	$0 - 0.03$	$0 + 0.03$	$\frac{1}{2} + 0.03$	$\frac{1}{2} - 0.03$	$\pm 0.015$
		$y$ :	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	$\frac{1}{4}$	$\pm 0.025$
		$z$ :	$\frac{1}{2} + 0.05$	$\frac{1}{2} - 0.05$	$0 + 0.05$	$0 - 0.05$	$\pm 0.015$
	O(2)	$x$ :	$\frac{1}{2} + 0.05$	$\frac{1}{2} - 0.05$	$\frac{3}{4} - 0.05$	$\frac{1}{4} + 0.05$	$\pm 0.005$
		$y$ :	$0 - 0.03$	$0 - 0.03$	$\frac{1}{2} - 0.03$	$\frac{1}{2} - 0.03$	$\pm 0.015$
		$z$ :	$\frac{1}{2} + 0.06$	$\frac{1}{2} + 0.06$	$\frac{3}{4} - 0.06$	$\frac{1}{4} - 0.06$	$\pm 0.015$
	O(3)	$x$ :	$\frac{1}{2} + 0.05$	$\frac{1}{2} - 0.05$	$\frac{3}{4} - 0.05$	$\frac{1}{4} + 0.05$	$\pm 0.005$
		$y$ :	$\frac{1}{2} + 0.07$	$\frac{1}{2} + 0.07$	$0 + 0.07$	$0 + 0.07$	$\pm 0.015$
		$z$ :	$\frac{1}{2} + 0.06$	$\frac{1}{2} + 0.06$	$\frac{3}{4} - 0.06$	$\frac{1}{4} - 0.06$	$\pm 0.015$

<sup>a)</sup> This specimen is not spherical, so that the value of  $H_{c1}(0)$  quoted is only approximate.  
<sup>b)</sup> Hall coefficient appeared to be affected by magnetic history of specimen at liquid helium temperature.

Nr. 1  
(Res)  
1a  
b2a  
b3  
45a  
b\* The  
cool  
\*\* In n  
[65J]

Nr. 1A-8 BaTiO<sub>3</sub>, Barium titanate

(Responsible authors for this section are as follows: IKEDA, NAKAMURA, NOMURA, SAWAGUCHI, SHIOZAKI and TOYODA, abbreviated as INANO-SASHITO).

1a	The anomalous dielectric properties of BaTiO <sub>3</sub> were discovered on ceramic specimens independently by WAINER and SOLOMON in 1942, by OGAWA in 1944 and by WUL in 1945. The ferroelectric activity of BaTiO <sub>3</sub> was reported independently by von HIPPEL and co-workers in 1944 and by WUL in 1946. The structural change associated with the cubic-tetragonal phase transition was observed, by means of x-rays, by MEGAW in 1945, independently of the above dielectric studies.					42W1, 4401, 45W1 44V2 46W2 45M1																																
b	<table border="1"> <thead> <tr> <th>phase</th><th>IV<sup>a)</sup></th><th>III<sup>a)</sup></th><th>II<sup>b)</sup></th><th>I<sup>b)</sup></th><th></th></tr> <tr> <th>state</th><th>F<sup>a)</sup></th><th>F<sup>a)</sup></th><th>F<sup>c)</sup></th><th>P<sup>b)</sup></th><th></th></tr> <tr> <th>crystal system</th><th>rhombo-hedral<sup>a)</sup></th><th>ortho-rhombic<sup>a)</sup></th><th>tetragonal<sup>b)</sup></th><th>cubic<sup>b)</sup></th><th>hexagonal<sup>d)*</sup></th></tr> <tr> <th>space group</th><th>R3m-C<sub>3v</sub><sup>a)</sup></th><th>Amm2-C<sub>2v</sub><sup>a)</sup></th><th>P4mm-C<sub>4v</sub><sup>b)</sup></th><th>Pm3m-O<sub>h</sub><sup>b)</sup></th><th>C63/mmc-D<sub>6h</sub><sup>d)</sup></th></tr> </thead> <tbody> <tr> <td><math>\Theta</math></td><td>— 90<sup>a)</sup></td><td>5<sup>a)</sup></td><td>120<sup>b)**</sup></td><td>1460<sup>d)</sup></td><td>°C</td><td></td></tr> </tbody> </table> <p> <math>P_s \parallel [001]</math> in phase II (along [100] of phase I).  <math>P_s \parallel [001]</math> in phase III (along [110] of phase I).  <math>P_s \parallel [111]</math> in phase IV (along [111] of phase I).  The directions of <math>P_s</math> are illustrated along with lattice distortions in Fig. 140.  <math>T_{melt} = 1618</math> °C.  Tetragonal form (phase II): <math>\rho = 6.02 \cdot 10^3</math> kg m<sup>-3</sup> (calculated from lattice constants)  <math>a = 3.9920</math> Å, <math>c = 4.0361</math> Å at 20 °C.  Transparent, light brown.  Hexagonal form: <math>a_{hex} = 5.735</math> Å, <math>c_{hex} = 14.05</math> Å at RT.  <math>\rho = (6.1 \pm 0.1) \cdot 10^3</math> kg m<sup>-3</sup>. </p>						phase	IV <sup>a)</sup>	III <sup>a)</sup>	II <sup>b)</sup>	I <sup>b)</sup>		state	F <sup>a)</sup>	F <sup>a)</sup>	F <sup>c)</sup>	P <sup>b)</sup>		crystal system	rhombo-hedral <sup>a)</sup>	ortho-rhombic <sup>a)</sup>	tetragonal <sup>b)</sup>	cubic <sup>b)</sup>	hexagonal <sup>d)*</sup>	space group	R3m-C <sub>3v</sub> <sup>a)</sup>	Amm2-C <sub>2v</sub> <sup>a)</sup>	P4mm-C <sub>4v</sub> <sup>b)</sup>	Pm3m-O <sub>h</sub> <sup>b)</sup>	C63/mmc-D <sub>6h</sub> <sup>d)</sup>	$\Theta$	— 90 <sup>a)</sup>	5 <sup>a)</sup>	120 <sup>b)**</sup>	1460 <sup>d)</sup>	°C		<sup>a)</sup> 49K2, 49R1 <sup>b)</sup> 45M1 <sup>c)</sup> 46V1, 46W1 <sup>d)</sup> 55R1
phase	IV <sup>a)</sup>	III <sup>a)</sup>	II <sup>b)</sup>	I <sup>b)</sup>																																		
state	F <sup>a)</sup>	F <sup>a)</sup>	F <sup>c)</sup>	P <sup>b)</sup>																																		
crystal system	rhombo-hedral <sup>a)</sup>	ortho-rhombic <sup>a)</sup>	tetragonal <sup>b)</sup>	cubic <sup>b)</sup>	hexagonal <sup>d)*</sup>																																	
space group	R3m-C <sub>3v</sub> <sup>a)</sup>	Amm2-C <sub>2v</sub> <sup>a)</sup>	P4mm-C <sub>4v</sub> <sup>b)</sup>	Pm3m-O <sub>h</sub> <sup>b)</sup>	C63/mmc-D <sub>6h</sub> <sup>d)</sup>																																	
$\Theta$	— 90 <sup>a)</sup>	5 <sup>a)</sup>	120 <sup>b)**</sup>	1460 <sup>d)</sup>	°C																																	
2a	<p>Crystal growth: Flux method (flux KF<sup>a)</sup> or TiO<sub>2</sub>-rich melt<sup>b)</sup>).  Pulling method (top-seeded solution growth technique using excess TiO<sub>2</sub> as the solvent).  Melting method (with limited success).  Tab. 29; Fig. 141.</p>					51W2 51R1 48B3																																
b	<p>Crystal forms: For butterfly-type: Fig. 142.  For chunky type: Fig. 143.  For hexagonal form: Fig. 144.</p>					<sup>a)</sup> 54R1, <sup>b)</sup> 65S8 63L3 50V2																																
3	<p>Crystal structure of phase I: <math>Z = 1</math>. Tab. 30.  Crystal structure of phase II: <math>Z = 1</math>. Tab. 31.  Crystal structure of phase III: <math>Z = 2</math>. Tab. 32; Fig. 145, 146; Tab. 33.  Crystal structure of phase IV: <math>Z = 1</math>.  Crystal structure of hexagonal form: <math>Z = 6</math>. Tab. 34, 35; Fig. 147.</p>																																					
4	<p>Lattice constants of phase I, II, III, and IV:  Phase I: <math>a = 3.996</math> Å at 120 °C.  Phase II: <math>a = 3.9920</math> Å, <math>c = 4.0361</math> Å at 20 °C.  Phase III: <math>a = 3.990</math> Å, <math>b = 5.669</math> Å, <math>c = 5.682</math> Å at —10 °C.  Phase IV: <math>a = 4.001</math> Å, <math>\alpha = 89^\circ 51'</math> at —168 °C.  Thermal expansion: Fig. 148, 149; Tab. 36, 37; Fig. 150.  Lattice distortion due to <math>p</math>: Fig. 151.</p>					47M3 51R1 57S2 57J2																																
5a	<p>Dielectric constant: Fig. 152, 153, 154, 192.  Dielectric dispersion: Fig. 155 ... 159.  Further data from optical measurements: Fig. 201; Tab. 42.  Effect of <math>p</math> on <math>\kappa</math>: Fig. 160, 161, 162.  Phase diagram in regard to <math>p</math>: Fig. 163, 164.  Effect of <math>E_{bias}</math> on <math>\Theta_f</math>: <math>d\Theta_f/dE_{bias} = 1.43 \cdot 10^{-5}</math> °K V<sup>-1</sup> m;  on <math>\kappa</math>: Fig. 165.</p>					53M2																																
b	Non-linear dielectric properties: Fig. 166. $\xi = -5.5 \cdot 10^8$ J C <sup>-4</sup> m <sup>6</sup> , $\zeta = 1.7 \cdot 10^{10}$ J C <sup>-6</sup> m <sup>9</sup> .					53M2																																

\* The transition from the hexagonal form to the cubic one is very sluggish and the hexagonal form can be produced by rapid cooling from above 1460 °C.

\*\* In most papers this Curie point has been reported to be about 120 °C, but it seems to be about 130 °C for pure BaTiO<sub>3</sub> [65J2].

			14a
5c	Nr. 1A-8 BaTiO <sub>3</sub> , continued Spontaneous polarization: Fig. 167, 168, 169. Coercive field: Fig. 170, 171, 172. Effect of $p$ on $P_s$ : Fig. 173.		
d	Electrocaloric effect: Fig. 174. Pyroelectricity: Fig. 175.		
6a	Specific heat: Fig. 176, 177. Transition heat, transition entropy: Tab. 38.		
b	Thermal conductivity: Fig. 178, 179.		
7a	Piezoelectricity: Tab. 39, 40; Fig. 180 ... 183.		
b	Electrostriction: Fig. 184, 185.		
8a	Elastic compliances and stiffnesses: Tab. 41. See also Tab. 40. Fig. 186 ... 193.		
b	Non-linear elastic properties: Fig. 194.		
9a	Refractive indices: Fig. 195, 196, 197. Birefringence: Fig. 198, 199. Reflection and absorption: (i) Far-infrared region, Fig. 200, 201; Tab. 42. (ii) Infrared region, Fig. 202, 203, 204. (iii) Visible region, Fig. 205, 206, 207. (iv) Ultraviolet region, Fig. 208; Tab. 43; Fig. 209, 210, 211. For the effect of $E_{bias}$ on the absorption edge, see		
b	Linear electrooptic effect: Fig. 212 ... 215. Quadratic electrooptic effect: $(M_{11} - M_{12}) = (+ 0.13 \pm 0.02) \text{ m}^4 \text{ C}^{-2}$ at 408 ... 433 °K, measured at 6328 Å.	67G1	
d	Faraday rotation: Fig. 216; Tab. 44.	64G3	
e	Non-linear optical properties: Susceptibility for SHG (second harmonic generation) (relative values, see Sec. I C): $d_{15} = 35 \pm 3$ , $d_{31} = 37 \pm 3$ , $d_{33} = 14 \pm 1$ , determined with the Nd-doped CaWO <sub>4</sub> laser beam. Fig. 217.	64M2	
f	Raman scattering: Fig. 218.		
g	Luminescence: Fig. 219, 220.		
10	Conductivity of as-grown crystals and ceramics: The data vary from sample to sample depending on the purity and the method of preparation: only representative data are given here. Fig. 221 ... 225. Conductivity associated with doping or reduction (including PTC (Positive Temperature Coefficient) or resistivity: $d\rho/dT > 0$ ): Fig. 226 ... 230. Reference papers on PTC anomaly: Tab. 45. Piezoresistivity: Fig. 231, 232. For additional data, see  Breakdown strength: Fig. 233, 234. For additional data, see	59S1, 63M1, 67G4	
	Photoconductivity and photoemission: Fig. 235, 236. Other transport properties: In <i>n</i> -type single-domain crystals, the electron mobility is anisotropic at RT; $\mu_{\perp c} \approx 1.2 \cdot 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$ , and $\mu_c \approx 0.13 \cdot 10^{-4} \text{ m}^2 \text{ V}^{-1} \text{ sec}^{-1}$ at 26 °C. In <i>n</i> -type single-domain crystals, the energy separation ( $\Delta u = 10^{-2} \dots 10^{-1} \text{ eV}$ ) between the <i>c</i> -axis conduction band minima and the <i>a</i> -axis conduction band minima has been estimated vs. $T$ . In <i>n</i> -type single-domain crystals, the density-of-state mass $m^* = (6.5 \pm 2) m_0$ . Data are available on the Hall coefficient and conductivity of single domain crystals having donor concentrations of $N = 8.5 \cdot 10^{24} \text{ m}^{-3}$ and of $N = 2.5 \cdot 10^{28} \text{ m}^{-3}$ . Fig. 237. Seebeck-effect: Fig. 238.	58I3, 59F1, 64K3, 64U1 67B2 67B2 67B2	
12b	ESR: Tab. 46; Fig. 239 ... 243.	67B2	
c	Mössbauer effect: Fig. 244 ... 247.	67B2	
13b	Diffuse X-ray scattering: Fig. 248, 249, 250. Inelastic neutron scattering: Fig. 251.		

14a	Domain structure: Domains have been observed by various methods: polarized light <sup>a)</sup> , X-rays <sup>b)</sup> , electron microscope <sup>c)</sup> , etching method <sup>d)</sup> , powder pattern method <sup>e)</sup> , and decoration method <sup>f)</sup> . Fig. 252 ... 255.	<sup>a)</sup> 48M1, <sup>a)</sup> 49F1, 52M3 <sup>b)</sup> 63B13, <sup>c)</sup> 64N1, 65C3, <sup>c)</sup> 64L1 <sup>c)</sup> 62T1, 63B9, <sup>c)</sup> 67R4, 64T2, <sup>c)</sup> 66R5, 67R2 <sup>d)</sup> 55H2 <sup>e)</sup> 59P1 <sup>f)</sup> 66S8
b	Domain wall motion: Domain wall motion has been observed optically <sup>a)</sup> and by repeated differential etching <sup>b)</sup> . The domain shapes in motion depend on the applied field and temperature. <sup>c)</sup> Fig. 256.  The wall velocity is proportional to $\exp(-\delta/E)$ at relatively low field. $\delta$ = activation field for domain wall motion. Fig. 257 ... 267.	<sup>a)</sup> 59M2, 60S2 <sup>b)</sup> 63S13 <sup>c)</sup> 63S13  58M4, 59M3
15	Surface layer: The first suggestion about the existence of surface layers of BaTiO <sub>3</sub> crystals was made by KÄNZIG <sup>a)</sup> on the basis of electron diffraction studies of very small particles of BaTiO <sub>3</sub> <sup>b)</sup> . The dependence of the following quantities on the thickness of the crystals has been observed as evidence of the existence of surface layers: domain wall velocity <sup>c)</sup> , dielectric constant <sup>d)</sup> , optical absorption coefficient <sup>e)</sup> and electroluminescence spectra <sup>f)</sup> . Pyroelectric current was observed above the Curie point and discussed in connection with surface layers <sup>g)</sup> . A few models of surface layers have been proposed <sup>h)</sup> . According to TANAKA and HONJŌ <sup>i)</sup> , the surface layer, if it exists, seems to be very thin.	<sup>a)</sup> 55K1 <sup>b)</sup> 54A1 <sup>c)</sup> 56M4, 61M2, 65C1 <sup>d)</sup> 61S4, 62C3 <sup>e)</sup> 60C3 <sup>f)</sup> 58H1, 65B7, 66B6 <sup>g)</sup> 56C1 <sup>h)</sup> 56M4, 61F2, 59D3, 65C1 <sup>i)</sup> 64T2
16	Radiation damage: Fig. 268, 269.	
17	Energy band structure: Fig. 270.	

Tab. 29. BaTiO<sub>3</sub>. Solubility in KF solution. [54K1]

T	1000	1050	1100	1150	1200	1250	1300	°C
BaTiO <sub>3</sub>	4	6	9	12.5	17	22.5	28.5	mole %

Tab. 30. BaTiO<sub>3</sub>. Fractional coordinates of atoms in the unit cell of phase I. [52M2]

	x	y	z
Ba	0	0	0
Ti	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
O	$\frac{1}{2}$	$\frac{1}{2}$	0
	$\frac{1}{2}$	0	$\frac{1}{2}$
	0	$\frac{1}{2}$	$\frac{1}{2}$

Tab. 31. BaTiO<sub>3</sub>. Shift of atoms in fractional coordinates of phase II from the positions of phase I. [51K1], [55F1], [61E3]

$\delta z_{\text{Ti}}$	$\delta z_{\text{O}(1)}$	$\delta z_{\text{O}(2)}$	Ba $B_{11}$ $B_{33}$	Ti $B_{11}$ $B_{33}$	O(1) $B_{11}$ $B_{33}$	O(2) $B_{11}$ $B_{33}$	References
0.014	-0.032	0	0.48	0.13	0.13	0.48	51K1
0.014	-0.023	-0.014	0.273	0.152	0.334	0.267	55F1
0.015	-0.024	-0.020	0.27 0.28	0.53 0.21	0.90 0.08	0.60 0.49 0.07	61E3
0.012	-0.026	0	0.27 0.28	0.46 0.30	0.90 0.50	0.60 0.90 0.90	61E3

The positions of atoms in the unit cell are Ba at (0, 0, 0), Ti at ( $\frac{1}{2}$ ,  $\frac{1}{2}$ ,  $\frac{1}{2} + \delta z_{\text{Ti}}$ ), O(1) at ( $\frac{1}{2}$ ,  $\frac{1}{2}$ ,  $\delta z_{\text{O}(1)}$ ) and O(2) at ( $\frac{1}{2}$ , 0,  $\frac{1}{2} + \delta z_{\text{O}(2)}$ ).

Tab. 32.  $\text{BaTiO}_3$ . Fractional coordinates of atoms in the unit cell of phase III. [57S2]

	<i>x</i>	<i>y</i>	<i>z</i>
Ba	0	0	0
	0	$\frac{1}{2}$	$\frac{1}{2}$
Ti	$\frac{1}{2}$	0	$\frac{1}{2} + \delta z_{\text{Ti}}$
	$\frac{1}{2}$	$\frac{1}{2}$	$\delta z_{\text{Ti}}$
O(1)	0	0	$\frac{1}{2} + \delta z_{\text{O}(1)}$
	0	$\frac{1}{2}$	$\delta z_{\text{O}(1)}$
O(2)	$\frac{1}{2}$	$\frac{1}{2} + \delta y_{\text{O}(2)}$	$\frac{1}{2} + \delta z_{\text{O}(2)}$
	$\frac{1}{2}$	$\frac{1}{2} + \delta y_{\text{O}(2)}$	$\frac{1}{2} + \delta z_{\text{O}(2)}$
	$\frac{1}{2}$	$\frac{1}{2} - \delta y_{\text{O}(2)}$	$\frac{1}{2} + \delta z_{\text{O}(2)}$
	$\frac{1}{2}$	$\frac{1}{2} - \delta y_{\text{O}(2)}$	$\frac{1}{2} + \delta z_{\text{O}(2)}$

$\delta z_{\text{Ti}} = +0.010$ ;  $\delta z_{\text{O}(1)} = -0.010$ ;  $\delta z_{\text{O}(2)} = -0.013$ ;  
 $\delta y_{\text{O}(2)} = +0.003$ .

Tab. 33.  $\text{BaTiO}_3$ . Comparison of atomic shifts in phase III and phase II with respect to different origins. The coordinate of atoms of [55F1] and [57S2] are used for phase II and III, respectively. [57S2]

	Orthorhombic	Tetragonal
$\delta z$	Ti	Ba at (000)
	O(1)	+0.06 Å
	O(2)	-0.06 Å
	$\delta y_{\text{O}(2)}$	-0.07 Å
$\delta z$	$\delta z_{\text{O}(2)}$	±0.02 Å
	Ti	+0.13 Å
	Ba	+0.07 Å
	O(1)	+0.02 Å

Origin is chosen to give  $\delta z_{\text{O}(2)} = 0$

$\delta z$

Tab. 34.  $\text{BaTiO}_3$ . Fractional coordinates of atoms in the unit cell of hexagonal structure. [48B3]

2Ba(1) at (b),  
4Ba(2) at (f),  $z = 0.097$ ,  
2Ti(1) at (a),  
4Ti(2) at (f),  $z = 0.845$ ,  
6O(1) at (b),  $z = 0.522$ ,  
12O(2) at (k),  $z = 0.836$ ,  $z = 0.076$

Tab. 35.  $\text{BaTiO}_3$ . Interatomic distances of hexagonal structure. [48B3]

$O(1) - O(1)$	2.49 Å	in the shared face.
	= 3.25 Å	in the same layer but the atoms do not belong to the same shared face.
$O(2) - O(2)$	2.91 Å	
$O(1) - O(2)$	2.91 Å	
$Ti(2) - O(1)$	1.96 Å	
$Ti(2) - O(2)$	2.02 Å	
in the $\text{TiO}_6$ octahedra		
$O(2) - O(2)$	2.82 Å	in the same layer.
$O(2) - O(2)$	2.69 Å	between adjacent layers.
$Ti(1) - O(2)$	1.95 Å	

Tab. 36.  $\text{BaTiO}_3$ . Lattice constants and unit cell volume at various  $T$ . [51R1]

$T$ °C	<i>a</i> Å	<i>b</i> Å	<i>c</i> Å	<i>V</i> Å <sup>3</sup>
+ 20	3.9920	3.9920	4.0361	64.317
+ 4	3.9910	3.9911	4.0357	64.282
$\Theta_{\text{III-II}}$				
+ 4	4.0185	3.9860	4.0162	64.319
- 99	4.0170	3.9750	4.0150	64.093
$\Theta_{\text{IV-III}}$				
- 99	4.0015	4.0015	4.0020	64.079
- 160	3.9996	3.9996	3.9997	63.981

Accuracy of measurement below RT was  $\pm 0.0007$  Å.

Tab. 37.  $\text{BaTiO}_3$ . Linear thermal expansion coefficients along *a*, *b*, and *c* axes. [51R1]

$T$ °C	$\alpha_a$ $10^{-6} \text{ }^{\circ}\text{C}^{-1}$	$\alpha_b$ $10^{-6} \text{ }^{\circ}\text{C}^{-1}$	$\alpha_c$ $10^{-6} \text{ }^{\circ}\text{C}^{-1}$
+20 ... + 4	15.7	15.7	
+ 4 ... - 99	4.9	28.4	-0.9
-99 ... -160	7.8	7.8	8.2

Tab. 38.  $\text{BaTiO}_3$ . Transition heats and transition entropies

Transition	$\Delta Q_m$ cal mol <sup>-1</sup>	$\Delta S_m$ cal mol <sup>-1</sup> °K <sup>-1</sup>	References
IV → III	8 ± 2	0.04	52S5
	14.3	0.07	52V1
	12	0.06	52T1
III → II	22 ± 4	0.076	52S5
	15.5	0.054	52V1
	16	0.058	52T1
II → I	50 ± 5	0.125	52S5
	47	0.12	52V1
	47	0.12	48B1



Tab. 41. BaTiO<sub>3</sub> (single crystal and ceramics). Elastic constants. [66b]

	$s_{11}^E$	$s_{11}^D$	$s_{33}^E$	$s_{33}^D$	$s_{13}^E$	$s_{13}^D$	$s_{12}^E$	$s_{12}^D$	$s_{34}^E$	$s_{34}^D$	$s_{44}^E$	$s_{44}^D$	$T$ °C	References
10 <sup>-18</sup> m <sup>3</sup> N <sup>-1</sup>														
single crystal	9.26 11.2	7.25 8.05	15.7 10.8	10.8 7.1	-2.35 -2.61 -2.7	-3.15 -2.98 -3.0	-5.24 -2.85 -2.9	-3.26 -1.95 -1.9	18.4 23.3 22.8	12.4 18.3 17.5	8.84 22.3 23.6	25 25 25	50C2 51B1 58B2	
ceramics	8.55 9.1	8.18 8.7	8.93 9.5	6.76 7.1	-2.61 -2.7	-2.98 -2.9	-1.95 -1.9	-1.95 22.8	18.3 17.5	22.3 23.6	25 25	56B3 64b1		
	$c_R^E$	$c_R^D$	$c_{33}^E$	$c_{33}^D$	$c_{13}^E$	$c_{13}^D$	$c_{34}^E$	$c_{34}^D$	$c_{44}^E$	$c_{44}^D$	$c_{66}$			
single crystal	275.1	282.6 206	164.9 162	178.1 146	179.0 189	186.5 171	151.6 66	141.6 77.5	54.34 71.0	80.64 42.9	113.1 54.6	25	66b1, 58B2 51B1	
ceramics	166 150 165.6	168 150	162 146	189 171 180.7	76.6 68	78.2 68	77.5 66	57	42.9 44 42.48	44.8 57 53.02	45.65	25 25 25	56B3 64b1 55HS	

Tab. 42 ... 45 see page 58

Tab. 46. BaTiO<sub>3</sub>. Summary of the ESR parameters for various paramagnetic centers in doped BaTiO<sub>3</sub>.

Paramagnetic center	Site	$S$	$\nu$	GHz	$T$ °K	$g$ -factor	FS		HFS		Ref.	Literature
							$D$ , $E$ , $a$ , $F$ [10 <sup>-3</sup> m <sup>-1</sup> ]	$I$	$A$ , $B$ [10 <sup>-4</sup> m <sup>-1</sup> ]	$I$		
Mn <sup>3+</sup>	Ti <sup>4+</sup>	5/2	(7)	9.3	78	2.0016 ± 0.0005	$D = 56 \pm 5$				5/2	6011
						2.0023 ± 0.0005	$D = 65 \pm 5$					
Ba <sup>2+</sup>						440	2.0009 ± 0.001	$a = 14 \pm 5$			5/2	6301
						RT	2.002 ± 0.001	$D = + (215 \pm 2)$ $a = + (16.76 \pm 0.94)$	$E = 0$			
						438	2.002 ± 0.001	$D = 0$ $a = +(12.11 \pm 0.94)$	$E = 0$			
									$\frac{ssA_{  }}{ssA_{\perp}} = - (77.4 \pm 0.6)$			6415
									$\frac{ssA_{  }}{ssA_{\perp}} = -(82.3 \pm 0.8)$			
									$\frac{ssA_{  }}{ssA_{\perp}} = -(79.3 \pm 0.4)$			6613 <sup>b)</sup>

$D_{\text{Ba}^+}$	$\sim 14$	$\sim 14$	$D = 0$	$E = 0$
438	$2.002 \pm 0.001$		$a = +(12.11 \pm 0.94)$	

Para-magnetic center	Site	$S$	$\nu$	GHz	$T$	g-factor	FS		HFS		Ref.	Literature
							$D, E, a, F, b [10^{-2} \text{ m}^{-1}]$	$I$	$A, B [10^{-2} \text{ m}^{-1}]$			
Fe <sup>+</sup>	Ti <sup>4+</sup>	5/2	(7)	5 ... 7.5	393,	2.003	$D = 0$				d) 59H5, 62R1 e) 63S2 <sup>a)</sup>	
				10, 16.3	433,		$a = 102 \pm 12$					
				300	2.0036 $\pm$ 0.002		$D = +929$	$E = 0$				
				276	2.0036 $\pm$ 0.002		$a = +91 \pm 20$					
				213	2.0036 $\pm$ 0.002		$D = -530 \pm 10$					
		7/2	(7)	2.0036 $\pm$ 0.002			$a = +105 \pm 20$				f) 64S3 <sup>b)</sup>	
				77	2.0036 $\pm$ 0.002		$D = -640 \pm 10$					
				173	2.003 $\pm$ 0.002		$E = 0 \pm 1.3$					
				173	2.003 $\pm$ 0.002		$D = 0$	$E = 0$				
							$a = +115 \pm 10$					
Co <sup>+</sup>	Ti <sup>4+</sup>	1/2	(3)	9	4	4.347 (isotropic)					g) 67Z2	
Gd <sup>3+</sup>	Ba <sup>2+</sup>	7/2	(8)	12, 18	300	1.995 $\pm$ 0.003	$b_{30}$	$b_{40}$	$b_{60}$		62R1	
				425	1.995 $\pm$ 0.003		$-293.6 \pm 1.0$	$+4.0 \pm 1.0$	$1.6 \pm 1.0$			
	Ti <sup>4+</sup>			10	RT	1.992	—	$\approx 6$	—		64T1	
				436	1.992		—	24	$\pm 0.9$	$-3.7 \pm 2.8$	66T3	
Pt <sup>+</sup>	Ti <sup>4+</sup>	1/2	(3)	10	4	$g_{  }$	$g_{\perp}$	$23.3 \pm 0.4$	$-1.8 \pm 0.4$			
				78		$1.950 \pm 0.005$	$2.459 \pm 0.003$				66S21	
Electron	oxygen vacancy			10	55	1.935 $\pm$ 0.005	$2.51 \pm 0.02$					
						1.911					63S11, 66T2, 67T3	

<sup>a)</sup> Temperature dependence of  $D_s$  in the tetragonal phase is linear. [65V4].

<sup>b)</sup> Forbidden transition lines ( $\Delta M = \pm 1, \Delta m = \pm 1$ ) are observed. [63O], [64T], [66T].

<sup>c)</sup> Temperature dependence of  $^{ss}A$ . [67Z].

<sup>d)</sup> Fe<sup>+</sup> spectra are studied with a d.c. bias electric field near transition temperature from cubic to tetragonal phase and from tetragonal to orthorhombic phase. [64S3].

<sup>e)</sup> Forbidden transition lines ( $\Delta M = 2, 3, 4, 5$ ) are observed in the rhombohedral phase. [65G].

<sup>f)</sup> Fe<sup>+</sup> spectra due to the oxygen vacancy;  $g_{||} \approx 2, g_{\perp} = 6.0 \pm 0.1$  at 77 °K. [64D].

<sup>g)</sup> Hyperfine structure of an electron captured by an oxygen vacancy. [64G].

<sup>1)</sup> Mn<sup>+</sup> ion takes the place of Ti<sup>4+</sup> lattice site in ceramics, while it takes the place of Ba<sup>2+</sup> in a single crystal.

<sup>2)</sup> Positive  $a$  is assumed.

<sup>3)</sup> Fe<sup>+</sup> spectra in a single-domain specimen.

Tab. 42.  $\text{BaTiO}_3$ ,  $\text{SrTiO}_3$ ,  $\text{TiO}_2$ ,  $\text{KTaO}_3$ . Dispersion parameters calculated from the Kramers-Kronig analysis [62S11]. See Fig. 201

	$\chi' = \infty + \sum_i 4\pi \rho_i \nu^2 \frac{\nu_i^2 - \nu^2}{(\nu_i^2 - \nu^2)^2 + \gamma_i^2 \nu^2}$	$\chi'' = \sum_i 4\pi \rho_i \nu_i^2 \frac{\gamma_i \nu}{(\nu_i^2 - \nu^2)^2 + \gamma_i^2 \nu^2}$	$\text{TiO}_2$ Ordinary ray	$\text{KTaO}_3$
$\lambda_1; \nu_1$	20.4; 491	18.4; 544	20.0; 500	18.2 $\pm$ 0.2; 549 $\pm$ 6
$\gamma_1/\nu_1$	$0.059 \pm 0.002$	$0.049 \pm 0.002$	$0.044 \pm 0.004$	$0.043 \pm 0.009$
$4\pi \rho_1$	$0.60 \pm 0.03$	$1.56 \pm 0.06$	$2.0 \pm 0.2$	$2.4 \pm 0.5$
$\lambda_2; \nu_2$	54.8; 183	$56.3 \pm 0.5$ ; 178 $\pm$ 2.0	25.8; 388	49.8; 200.8
$\gamma_2/\nu_2$	$0.030 \pm 0.006$	$0.039 \pm 0.004$	$0.058 \pm 0.006$	$0.055 \pm 0.011$
$4\pi \rho_2$	$2.2 \pm 0.4$	$3.6 \pm 0.4$	$1.08 \pm 0.1$	$7.6 \pm 1.5$
$\lambda_3; \nu_3$	$296 \pm 8$ ; $33.8 \pm 0.9$	$114.3 \pm 1.1$ ; $87.7 \pm 0.9$	$54.8 \pm 0.5$ ; $183 \pm 1.8$	$107.5 \pm 2.0$ ; $93.0 \pm 2.0$
$\gamma_3/\nu_3$	$2.5 \pm 0.1$	$0.5 \pm 0.1$	$0.19 \pm 0.01$	$0.5 \pm 0.1$
$4\pi \rho_3$	$1830 \pm 70$	$311 \pm 62$	$81.5 \pm 4.1$	$163 \pm 33$

Resonance wavelength  $\lambda_i$  in  $10^{-8}$  m; resonance frequency  $\nu_i$  in  $10^2$  m $^{-1}$ ; width  $\gamma_i$ ; strength  $4\pi \rho_i$ .

Tab. 43.  $\text{BaTiO}_3$ ,  $\text{SrTiO}_3$ ,  $\text{TiO}_2$ . Energies of fundamental absorption edges (in eV) at RT. [65C2]

	$E_0$	$A_1$	$A_2$	$A_3$	$B_1$	$B_2$	$C_1$	$C_2$	$D$	$E$	
$\text{SrTiO}_3$	3.2	4.00	4.86	5.5	6.52	7.4	9.2	9.9	12.5	15.3	eV
$\text{BaTiO}_3$	3.2	3.91	4.85		6.10	7.25	10.3	11.8	12.8	15	eV
$\text{TiO}_2$ ( $E \perp c$ )	3.97	5.52			6.50	7.64	8.53	9.24	11	14.1	eV

Tab. 44.  $\text{BaTiO}_3$ ,  $\text{SrTiO}_3$ ,  $\text{KTaO}_3$ ,  $\text{KTa}_{0.35} \text{Nb}_{0.65} \text{O}_3$  (KTN),  $\text{TiO}_2$ . Band gap energies  $\hbar \omega_g$  (in eV). [67B1]. See Fig. 46, 103, 216, 430.  $F_1$ ,  $F_2$ : different dispersion functions  $F_i(\omega/\omega_g)$ , see [67B1]

	$\text{SrTiO}_3$		$\text{BaTiO}_3$		$\text{KTaO}_3$		$\text{KTN}$		$\text{TiO}_2$		
	296 °K	77 °K	403 °K	296 °K	77 °K	296 °K	77 °K	296 °K	296 °K		
Faraday rotation $\hbar \omega_g$ for $F_1$	3.40	3.43	3.25	3.77	3.79	3.54	3.62				eV
Faraday rotation $\hbar \omega_g$ for $F_2$	3.21	3.26	3.11	3.62	3.65	3.36	3.37				eV
Energy of reflectivity peak or shoulder	3.20	—	3.20	—	—	3.70	—				eV
Energy of electroreflectance singularity	—	—	3.20	3.57	—	3.60	3.00				eV
$\hbar \omega_g$ from absorption data	3.40	—	—	3.80	—	—	3.30				eV
Energy at which absorption coefficient $\alpha \approx 10^4 \text{ cm}^{-1}$	3.37	—	3.26	3.75	—	3.45	—				eV
				3.79	—	3.45	3.18				eV

Tab. 45.  $\text{BaTiO}_3$  (reduced or doped). List of reference papers on PTC anomaly

Materials (dopants)	References	Materials (dopants)	References
Single crystal $\text{BaTiO}_3$ : reduced	57H1, 63K3, 64I4, 64G4, 65M1, 65U2 64B11	Ceramics $\text{BaTiO}_3$ $\text{BaTiO}_3$ : La	63H5, 65U2 59S1, 63T3, 64J1, 65M1
$\text{BaTiO}_3$ : Nb		$\text{BaTiO}_3$ : Ce $\text{BaTiO}_3$ : Sm $\text{BaTiO}_3$ : Gd $\text{BaTiO}_3$ : Sb (Ba-Sr) $\text{TiO}_3$ (Ba-Sr) $\text{TiO}_3$ : La $\text{BaTiO}_3$ : Sr, Ce, Sn $\text{BaTiO}_3$ : Sr, Ca, Sn $\text{BaTiO}_3$ : Sr, Bi $\text{BaTiO}_3$ : Mg, Ce $\text{BaTiO}_3$ : Zr, Ce $\text{BaTiO}_3$ : Si, Ce	63T3 63G5 65U2 65A3 61H5, 65A3 59S1, 61T1, 63T3 61S1 61S1 63T3 61S1 61S1 61S1

Nr. 1A-	
1a	F Si
b	pl st cr sp
2a	G Cl
3	C P
4	T L
5a	D a: C
6a	S
c	A T
7a	F
9a	E I: F
12b	E
14a	I
16	F
T	P:
	-
	-
	• Phase

Kronig

1 ± 6  
093  
11

0 ± 2.0

h  $4\pi\varrho_i$ (in eV).  
[67B1]

K

2 eV

7 eV

0 eV

0 eV

18 eV

Nr. 1A-9 PbTiO<sub>3</sub>, Lead titanate

1a	Ferroelectric activity was reported independently by SHIRANE et al. and by SMOLENSKII in 1950.			50S4 50S6
b	phase	III <sup>b</sup> )*	II <sup>a</sup> )	I <sup>a</sup> )
	state		F <sup>a</sup> )	P <sup>a</sup> )
	crystal system		tetragonal <sup>c</sup> )	cubic <sup>a</sup> )
	space group		P4mm-C <sub>4v</sub> <sup>1</sup>	Pm3m-O <sub>h</sub> <sup>1</sup>
	$\Theta$	-100 <sup>b</sup> )	490 <sup>a</sup> )	°C
	$a = 3.904$ Å, $c = 4.152$ Å at RT (in phase II).			46M2
2a	Crystal growth: KF flux method; PbCl <sub>2</sub> flux method.			58K1, 52N2
b	Crystal form: Fig. 271.			
3	Crystal structure: Positional parameters: Tab. 47, 48. Projection of crystal structure: Fig. 272, 273.			
4	Thermal expansion: Fig. 274 ... 280. Dependence of lattice parameters on hydrostatic pressure: Fig. 281.			
5a	Dielectric constants: Fig. 282. Small dielectric anomaly was observed at about -100 and -150 °C. Curie-Weiss constant: $C = 1.1 \cdot 10^5$ °K (single crystal).			56K2 62B4
6a	Specific heat: Fig. 283.			
	II-I			
	$\Delta Q_m$	1150	cal mol <sup>-1</sup>	51S7
	$\Delta S_m$	1.6	cal °K <sup>-1</sup> mol <sup>-1</sup>	51S7
c	Thermal conductivity: Fig. 284.			
7a	Piezoelectric properties: Tab. 49.			
9a	Birefringence: Fig. 285. Infrared absorption: Fig. 286, 287. Frequencies of infrared modes: Tab. 50.			
12b	ESR: Tab. 51.			
14a	Domain structures were observed by polarized light.			52N2, 58K1, 59K1
16	Radiation damage: Fig. 288.			

Tab. 47. PbTiO<sub>3</sub>. Positional parameters of atoms at RT. [56S5]

	x	y	z
Pb	0	0	0
Ti	$\frac{1}{2}$	$\frac{1}{2}$	0.540
O(1)	$\frac{1}{2}$	$\frac{1}{2}$	0.112
O(2)	$\frac{1}{2}$	0	0.612
	0	$\frac{1}{2}$	0.612

Tab. 48. PbTiO<sub>3</sub>. Bond lengths in Å at RT (phase II) and at 490 °C (phase I) [56S5]. O(1)+ represents the O(1) ion closer to, O(1)- that further away from Ti. Similarly O(2)+ is closer to Pb

phase	II (at RT)	I (at 490 °C)
Ti-O(1)+	1.78	1.89
Ti-O(1)-	2.38	
Ti-O(2)	1.98	
Pb-O(1)	2.80	2.80
Pb-O(2)+	2.53	
Pb-O(2)-	3.20	

Phase transition II-III was reported to occur only if the cooling rate is extremely slow. [55K3]

Tab. 49.  $\text{PbTiO}_3$  (modified ceramics). Electromechanical constants at RT. [68U1]

Additive	$\text{PbNb}_{4/5}\text{O}_9$ 5.0 mol%	$\text{BiZn}_{1/2}\text{Ti}_{1/3}\text{O}_3$ 5.0 mol%	$\text{Bi}_{2/3}\text{Zn}_{1/3}\text{Nb}_{2/3}\text{O}_3$ 5.0 mol%	
<i>a</i>	3.915	3.904	3.911	
<i>c</i>	4.104	4.148	4.133	A
<i>c/a</i>	1.049	1.062	1.057	A
<i>e</i>	7.19	7.68	7.12	
porosity	0.105	0.036	0.10	$10^3 \text{ kg m}^{-3}$
$\Theta$	466	524	494	°C
$\tilde{\nu}_{11}$	—	195	244	
$\tilde{\nu}_{33}$	226	147	203	
$d_{31}$	10	3.9	7.4	$10^{-12} \text{ C N}^{-1}$
$d_{33}$	37	37	47	$10^{-12} \text{ C N}^{-1}$
$g_{s1}$	5.2	3.0	4.1	$10^{-8} \text{ m}^2 \text{ C}^{-1}$
$g_{s3}$	16	28	28	$10^{-8} \text{ m}^2 \text{ C}^{-1}$
$s_{11}^E$	1.2	1.2	1.1	$10^{-11} \text{ m}^2 \text{ N}^{-1}$
$s_{33}^E$	1.1	0.95	1.1	$10^{-11} \text{ m}^2 \text{ N}^{-1}$
$Q_{\text{mech}}$ for $s_{11}$	-336	54	326	
for $s_{33}$	71	74	76	
$k_{15}$	—	0.40	0.36	
$k_{31}$	0.068	0.031	0.052	
$k_{33}$	0.23	0.32	0.35	

Tab. 50.  $\text{PbTiO}_3$ . Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Ti-O stretch)	$\tilde{\nu}_2$ (Ti-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Ti-O bend)	$\tilde{\nu}_4$ (cation-TiO <sub>3</sub> lattice mode)
530 ( $E_u, A_1$ )	400 ( $B_1, E_u$ )	220 ( $E_u, A_1$ ) 172	83 ( $E_u, A_1$ )

Tab. 51.  $\text{PbTiO}_3$ . g-factors at RT. [64G1]

Paramagnetic center	Site	$S$	$\mathcal{H}$	GHz	$T$ °K	g-factor	
						$g_{\parallel}$	$g_{\perp}$
Fe <sup>3+</sup>	Ti <sup>4+</sup>	1/2*	(2)	8.8	RT	$2.009 \pm 0.005$	$5.97 \pm 0.02$

The spectrum up to 300 °C and down to -120 °C did not show any fundamental change.

#### Nr. 1A-10 CaZrO<sub>3</sub>, Calcium zirconate

1	A few physical properties of CaZrO <sub>3</sub> were studied in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be orthorhombic with the cell dimensions $a = 5.587 \text{ \AA}$ , $b = 8.008 \text{ \AA}$ , $c = 5.758 \text{ \AA}$ at RT.						
4	Linear thermal expansion: $\alpha = 8.55 \cdot 10^{-6} \text{ }^{\circ}\text{C}^{-1}$ between 23 °C and 223 °C; $\alpha = 9.53 \cdot 10^{-6} \text{ }^{\circ}\text{C}^{-1}$ between 223 °C and 333 °C for ceramics of bulk density $\varrho = 4.95 \cdot 10^3 \text{ kg m}^{-3}$						55C1
9	Infrared absorption: Fig. 289, 290; Tab. 52.						65B10

Tab. 52. CaZrO<sub>3</sub>. Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO <sub>3</sub> lattice mode)
515 ( $B_1, B_2, A_1$ )	340 ( $B_1, B_2, A_1$ ) (377) (418)	228 ( $B_1, B_2, A_1$ ) 186	153 ( $B_1, B_2, A_1$ ) 96

\* The fictitious spin is  $\frac{1}{2}$  [64G1].

Nr. 1A-11 SrZrO<sub>3</sub>, Strontium zirconate

1	A few physical properties of SrZrO <sub>3</sub> were studied in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be pseudo-cubic with $a' = 4.099 \text{ \AA}$ at RT.	57R2
4	Linear thermal expansion: $\alpha = 8.75 \cdot 10^{-6} \text{ ^\circ C}^{-1}$ between 23 °C and 320 °C; $\alpha = 9.34 \cdot 10^{-6} \text{ ^\circ C}^{-1}$ between 320 °C and 700 °C for ceramics of bulk density $\rho = 5.00 \cdot 10^3 \text{ kg m}^{-3}$ .	65B10
9	Infrared absorption: Fig. 291, 292; Tab. 53.	

Tab. 53. SrZrO<sub>3</sub>. Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetry of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO <sub>3</sub> lattice mode)
522 ( $B_1, B_2, A_1$ ) (357) (379)	325 ( $B_1, B_2, A_2$ )	240 ( $B_1, B_2, A_1$ )	143 ( $B_1, B_2, A_1$ )

Nr. 1A-12 BaZrO<sub>3</sub>, Barium zirconate

1	A few properties of BaZrO <sub>3</sub> were reported in comparison with those of some perovskite-type ferroelectrics. The crystal was reported to be cubic with the cell dimensions $a = 4.192 \text{ \AA}$ at RT.	57R2
4	Linear thermal expansion: $\alpha = 5.64 \cdot 10^{-6} \text{ ^\circ C}^{-1}$ between 23 °C and 214 °C; $\alpha = 6.54 \cdot 10^{-6} \text{ ^\circ C}^{-1}$ between 214 °C and 324 °C for ceramics of bulk density $\rho = 6.73 \cdot 10^3 \text{ kg m}^{-3}$ .	65B10
9	Infrared absorption: Fig. 293, 294; Tab. 54.	

Tab. 54. BaZrO<sub>3</sub>. Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO <sub>3</sub> lattice mode)
505 ( $F_{1u}$ )	— ( $F_{2u}$ )	210 ( $F_{1u}$ )	115 ( $F_{1u}$ )

Nr. 1A-13 PbZrO<sub>3</sub>, Lead zirconate

1a	Dielectric anomaly of PbZrO <sub>3</sub> associated with a phase transition was reported independently by ROBERT and by SMOLENSKII in 1950. Antiparallel ionic shifts on the (001) projection of crystal structure were found by SAWAGUCHI et al. in 1951. In the same year antiferroelectric double hysteresis loops were discovered by SHIRANE et al.. PbZrO <sub>3</sub> is the first compound in which double hysteresis loops were observed.	50R1, 50S7 51S3 51S8
b	phase	II <sup>a)</sup>
	state	A <sup>b)</sup>
	crystal system	orthorhombic <sup>c)</sup>
	space group	Pba2-C <sub>2v</sub> <sup>c)</sup>
	$\Theta$	230 °C <sup>a)</sup>
		$a = 5.87 \text{ \AA}, b = 11.74 \text{ \AA}, c = 8.20 \text{ \AA}$ at RT (in phase II). The cubic unit cell in phase I becomes pseudo-tetragonal in phase II. The pseudo-tetragonal cell constants $a'$ and $c'$ are related with the orthorhombic cell constants $a$ , $b$ and $c$ : $a = \sqrt{2} a'$ , $b = 2\sqrt{2} a'$ and $c = 2c'$ , where $a' = 4.15 \text{ \AA}$ , $c' = 4.10 \text{ \AA}$ at RT. Relation between the pseudo-tetragonal and orthorhombic cells: Fig. 295.
		51S3
a	Crystal growth: PbCl <sub>2</sub> flux method.	55J2

Figuren S. 271ff.

II 1 Oxide des Perowskit-Typs

					4
3	Nr. 1A-13 PbZrO <sub>3</sub> , continued Z = 8 (in phase II). The crystal is polar along the c axis and antipolar along the a axis in phase II. Fig. 295 shows schematically the shifts of Pb ions. Positional parameters and shifts from ideal perovskite positions: Tab. 55. Projection of ZrO <sub>6</sub> . Fig. 296, 297, 298. Bond distances between Zr and O: Fig. 299.			51S3, 57J4, 51S3 57J4	
4	Thermal expansion: Fig. 300 ... 303. $\alpha_a' \cong -0.05 \cdot 10^{-5} \text{ K}^{-1}$ and $\alpha_c' \cong 2.80 \cdot 10^{-5} \text{ K}^{-1}$ in phase II; $\alpha_a' \cong 1.10 \cdot 10^{-5} \text{ K}^{-1}$ in phase I, where $\alpha_a'$ and $\alpha_c'$ are the linear thermal expansion coefficients along the pseudo-tetragonal a' and c' axes, respectively.			52S1	
5a	Dielectric constants: Fig. 304. $C = 1.36 \cdot 10^5 \text{ F m}^{-2} \text{ K}^{-1}$ (determined with ceramics).			50R1	
c	Effect of pressure: Fig. 305. $(d\Theta_a/dP)_{P=0} = (4.1 \pm 0.2) \cdot 10^{-8} \text{ K N}^{-1} \text{ m}^2$ .			66R2	
6a	Critical field: Fig. 306.				
b	Specific heat: Fig. 307. For the transition II-I: $\Delta Q_m = 440 \text{ cal mol}^{-1}$ ; $\Delta S_m = 0.88 \text{ cal K}^{-1} \text{ mol}^{-1}$ .			52S2	
8	Thermal conductivity: Fig. 308.				
9a	Elastic compliances: Fig. 309.				
16	Birefringence: Fig. 310. Infrared absorption: Fig. 311, 312; Tab. 56.				
	Radiation damage: Fig. 313.				

Tab. 55. PbZrO<sub>3</sub> (ceramics). Atomic coordinates and shifts from ideal perovskite positions at RT. [57J4]

Atom	x	y	z	Wyckoff notation	Total shift Å
Pb'	0.706	0.127	0	4c	0.26
Pb''	0.706	0.127	0.500	4c	0.26
Zr'	0.243	0.124	0.250	4c	0.04
Zr''	0.243	0.124	0.250	4c	0.04
O(1)'	0.270	0.150	0.980	4c	0.35
O(1)''	0.270	0.100	0.480	4c	0.35
O(2)'	0.040	0.270	0.300	4c	0.53
O(2)''	0.040	0.270	0.750	4c	0.34
O(3)'	0	0.500	0.250	2b	0
O(3)''	0	0.500	0.800	2b	0.41
O(4)'	0	0	0.250	2a	0
O(4)''	0	0	0.800	2a	0.41

Tab. 56. PbZrO<sub>3</sub>. Wave numbers in  $10^2 \text{ m}^{-1}$  and symmetries of infrared modes of lattice vibration obtained from Kramers-Kronig analysis of the reflectance data at RT. [65P4]

$\tilde{\nu}_1$ (Zr-O stretch)	$\tilde{\nu}_2$ (Zr-O <sub>3</sub> torsion)	$\tilde{\nu}_3$ (O-Zr-O bend)	$\tilde{\nu}_4$ (cation-ZrO <sub>3</sub> lattice mode)
508 ( $E_u, A_1$ )	290 ( $B_1, E_u$ )	221 ( $E_u, A_1$ )	80 ( $E_u, A_1$ ) 34

Nr. 1A-14 PbHfO<sub>3</sub>, Lead hafnate

1a	A dielectric anomaly associated with a phase transition was observed, and the possibility of the antiferroelectricity was discussed by SHIRANE et al. in 1953.			
b	phase	III	II	I
state	(A)			P
crystal system	pseudo-tetragonal	tetragonal	cubic	
$\Theta$	163	215	°C	
	Lattice constants for the pseudo-tetragonal phase: $a' = 4.136 \text{ \AA}$ , $c'/a' = 0.991$ at RT.			
				53S3

7J4,

[57J4]

vibration

3S3

3S3

3S3

4	Thermal expansion: Fig. 314. Cubic thermal expansion coefficients: below 158 °C: $20 \cdot 10^{-6}$ deg $^{-1}$ ; above 215 °C: $27 \cdot 10^{-6}$ deg $^{-1}$ .	53S3																														
5a	Dielectric constant: Fig. 315. $C = 9.5 \cdot 10^4$ K (ceramics).	53S3																														
<b>Nr. 1A-15 BiFeO<sub>3</sub>, Bismuth ferrite</b>																																
1a	In 1960 <sup>a</sup> ) it was pointed out on the basis of x-ray studies of the solid solution, PbTiO <sub>3</sub> -BiFeO <sub>3</sub> , that BiFeO <sub>3</sub> could have a ferroelectric Curie point at high temperatures. The Curie point was estimated to be about 850 °C from studies of the same solid solution <sup>b</sup> ). Disagreement, however, exists among many experimental data reported so far, therefore reservation is necessary in deciding whether BiFeO <sub>3</sub> is ferroelectric or anti-ferroelectric. Antiferromagnetic anomaly in BiFeO <sub>3</sub> was observed by direct magnetic measurements at about 370 °C <sup>c</sup> ).	<sup>a</sup> )60F9, 60V2 <sup>b</sup> )61F3, 62F8 <sup>c</sup> )62S10, 63R1, 65I2																														
b	<table border="1"> <thead> <tr> <th>phase</th><th>IV</th><th>III</th><th>II</th><th>I</th></tr> </thead> <tbody> <tr> <td>state</td><td>(A) or (F), <math>A_{\text{magn}}^*</math></td><td>(A) or (F), <math>P_{\text{magn}}</math></td><td>(A) or (F), <math>P_{\text{magn}}</math></td><td>(P), <math>P_{\text{magn}}</math></td></tr> <tr> <td>crystal system</td><td>rhombohedral</td><td>rhombohedral</td><td>rhombohedral</td><td>cubic (possibly)</td></tr> <tr> <td>space group</td><td>R3m-C<sub>3v</sub><sup>**</sup></td><td></td><td></td><td></td></tr> <tr> <td><math>\Theta</math></td><td>370</td><td><math>\approx 575</math></td><td>850</td><td>°C</td></tr> </tbody> </table> <p><math>a = (3.962 \pm 0.001)</math> Å, <math>\alpha = 89^\circ 31' \pm 3'</math> at RT. Further references are available on unit cell parameters.</p>	phase	IV	III	II	I	state	(A) or (F), $A_{\text{magn}}^*$	(A) or (F), $P_{\text{magn}}$	(A) or (F), $P_{\text{magn}}$	(P), $P_{\text{magn}}$	crystal system	rhombohedral	rhombohedral	rhombohedral	cubic (possibly)	space group	R3m-C <sub>3v</sub> <sup>**</sup>				$\Theta$	370	$\approx 575$	850	°C	64T6 60V2, 60F6, 60Z2					
phase	IV	III	II	I																												
state	(A) or (F), $A_{\text{magn}}^*$	(A) or (F), $P_{\text{magn}}$	(A) or (F), $P_{\text{magn}}$	(P), $P_{\text{magn}}$																												
crystal system	rhombohedral	rhombohedral	rhombohedral	cubic (possibly)																												
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$\Theta$	370	$\approx 575$	850	°C																												
3	Crystal structure: From the x-ray diffraction studies, BiFeO <sub>3</sub> was found to belong to one of the five space groups: R 3, R $\bar{3}$ , R 32, R3m and R $\bar{3}$ m. Neutron diffraction studies suggested that BiFeO <sub>3</sub> belongs to the non-centrosymmetric space group R3m. The crystal structure can be regarded as consisting of alternating FeO <sub>6</sub> and BiO <sub>6</sub> trigonal pyramids: Fig. 316; Tab. 57. According to the electron diffraction study, BiFeO <sub>3</sub> belongs to the non-centrosymmetric space group R3m at RT. Atomic coordinates: Tab. 58. The space group R3m was, however, rejected by SMOLENSKII et al., because it does not satisfy the conditions for the existence of weak ferromagnetism. The magnetic structure of BiFeO <sub>3</sub> was proved to be G-type by the neutron diffraction experiments. Fig. 317, 318.	60Z2 63K5 64T6 64S9 63K5																														
4	Unit cell parameters: Fig. 319, 320. See also	66R8, 64T5																														
5a	Dielectric constant: Fig. 321, 322, 323. No reliable data on the dielectric constant in the high temperature region near 850 °C are available.																															
11	Magnetic susceptibility: Fig. 324. At RT, no spontaneous magnetic moment was observed in the fields up to 22 kOe.																															
12c	Mössbauer effect: Fig. 325, 326.																															
17	Calculations of the internal electric fields and their gradients in BiFeO <sub>3</sub> crystals were made on the basis of an ionic model.	67T7																														
Tab. 57. BiFeO <sub>3</sub> . Values of the interatomic distances [Å]. [63K5]. See Fig. 316. See also [64T6]																																
	<table border="1"> <thead> <tr> <th></th><th>520 °C</th><th>20 °C</th></tr> </thead> <tbody> <tr> <td>Bi-Fe (A)</td><td>3.841</td><td>3.857</td></tr> <tr> <td>Bi-Fe (B)</td><td>3.006</td><td>2.994</td></tr> <tr> <td>Bi-O (C)</td><td>2.903</td><td>2.907</td></tr> <tr> <td>Bi-O (D)</td><td>2.680</td><td>2.693</td></tr> <tr> <td>Fe-O (F)</td><td>2.233</td><td>2.214</td></tr> <tr> <td>Fe-O (G)</td><td>1.754</td><td>1.774</td></tr> <tr> <td>O-O (H)</td><td>2.841</td><td>2.859</td></tr> <tr> <td>O-O (K)</td><td>2.800</td><td>2.800</td></tr> <tr> <td>O-O (L)</td><td>2.680</td><td>2.724</td></tr> </tbody> </table>		520 °C	20 °C	Bi-Fe (A)	3.841	3.857	Bi-Fe (B)	3.006	2.994	Bi-O (C)	2.903	2.907	Bi-O (D)	2.680	2.693	Fe-O (F)	2.233	2.214	Fe-O (G)	1.754	1.774	O-O (H)	2.841	2.859	O-O (K)	2.800	2.800	O-O (L)	2.680	2.724	
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<p>* This state is presumably weak ferromagnetic. [66Y2] ** See subsection 3.</p>																																

Tab. 58. BiFeO<sub>3</sub>. Atomic coordinates. [64T6]

Atom	x	y	z
Bi	0.0337	0.0337	0.0337
Fe	0.5000	0.5000	0.5000
O(1)	-0.0280	0.5000	0.5000
O(2)	0.5000	-0.0280	0.5000
O(3)	0.5000	0.5000	-0.0280

Nr. 1A-16  $KIO_3$ , Potassium iodate

1a	Ferroelectric behavior in $KIO_3$ was reported by HERLACH in 1961.						
b	phase	V <sup>a)</sup>	IV <sup>a)</sup>	III <sup>a)</sup>	II <sup>a)</sup>	I <sup>a)</sup>	
	state		F <sup>a)</sup>	F <sup>a)</sup>	F <sup>a)</sup>	P <sup>a)</sup>	
	crystal system			trigonal <sup>b)*</sup>		trigonal <sup>a)</sup>	
	$\Theta$	-190 <sup>a)</sup>	-18, -10 <sup>a)**</sup>	70 <sup>a)</sup>	212 <sup>a)</sup>	°C	
	$T_{melt}$	= 560 °C.					
	$\rho$	= $3.9791 \cdot 10^3 \text{ kg m}^{-3}$ .					
	1)	A different value, 3.802, is also given in the same reference.					
		$a = (4.410 \pm 0.005) \text{ \AA}$ $\alpha = 89.41^\circ$ at RT, adopting trigonal system.					
		$a = 8.921 \text{ \AA}$ , $b = 8.916 \text{ \AA}$ , $c = 8.885 \text{ \AA}$ , $\alpha \cong \beta \cong \gamma \cong 90^\circ \pm 30'$ at RT, adopting triclinic system.					
		Transparent					
2a	Hydrothermal method: Fig. 327. Growth from the supersaturated solution with 10 ... 14% $HIO_3$ at a constant temperature: Fig. 328.						61H3 27m1
3	$Z = 1$ in phase III, adopting trigonal system. $Z = 8$ in phase III, adopting triclinic system.						61H3 65F3
4	Lattice deformation: $a = [4.44 + 0.00022 (T - 220)] \text{ \AA}$ , $\alpha = 89^\circ 20' - 0.09 (T - 220)'$ in phase I ( $T$ in °C).						61H3
5a	Dielectric constants: Fig. 329, 330.						66H17
c	Spontaneous polarization: Fig. 331.						61H3
9a	Absorption edge: Fig. 332.						67V2
12a	NMR: Fig. 333.						61H3

## 1B Complex perovskite-type oxides

Nr. 1B1-i  $(K_{1/2}Bi_{1/2})TiO_3$ , Potassium bismuth titanate

1a	Ferroelectricity in $(K_{1/2}Bi_{1/2})TiO_3$ was found by SMOLENSKII and AGRANOVSKAYA in 1959.						
b	phase	III	II	I			59S6
	state	(F)	(A)	P			
	crystal system	tetragonal	pseudo-cubic	cubic			62I5
	space group			Pm3m-O <sub>h</sub>			
	$\Theta$	270	410,380 <sup>a)</sup>	°C			
	$a = (3.913 \pm 0.003) \text{ \AA}$ , $c = (3.993 \pm 0.003) \text{ \AA}$ at RT.						<sup>a)</sup> 60S6
3	Crystal structure: Disordered perovskite.						62I5
4	Lattice distortion: Fig. 334. Thermal expansion: Fig. 335.						
5a	Dielectric constant: Fig. 336.						

Nr. 1B1-ii  $(Na_{1/2}Bi_{1/2})TiO_3$ , Sodium bismuth titanate

1a	Ferroelectricity in $(Na_{1/2}Bi_{1/2})TiO_3$ was found by SMOLENSKII and AGRANOVSKAYA in 1959.						59S6
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\* Various crystal systems have been proposed: trigonal [60S5], triclinic [65F3].  
\*\* -10 °C on heating, -18 °C on cooling.

1b	phase	III	II	I	
	state	F	(A)	P	
	crystal system	rhombohedral	pseudo-cubic	cubic	62I5
	space group			Pm3m-O <sub>b</sub> <sup>1</sup>	
	$\Theta$	$\approx 200^\circ$	320	°C	60S6
	$a = (3.891 \pm 0.002) \text{ \AA}$ , $\alpha = 89^\circ 36' \pm 3'$ at RT.				
3	Crystal structure: Disordered perovskite.				62I5
4	Thermal expansion: Fig. 337.				
5a	Dielectric constant: Fig. 338.				
c	Spontaneous polarization and coercive field: $P_s \approx 8.0 \cdot 10^{-2} \text{ C m}^{-2}$ ; $E_c \approx 14 \cdot 10^2 \text{ kV m}^{-1}$ at 116 °C.				60S6

Nr. 1B2-i  $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$ 

1a	Antiferroelectric properties of $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$ were discovered by SMOLENSKII et al. in 1959.					59S7
b	phase	II	I			
	state	A	P			
	crystal system	orthorhombic	cubic			62Z1
	space group	C222 <sub>1</sub> -D <sub>2</sub> <sup>5</sup>				
	$\Theta$	38	°C			
	$a = 22.74 \text{ \AA}$ , $b = 22.79 \text{ \AA}$ , $c = 15.90 \text{ \AA}$ at RT. Orthorhombic unit cell: see Fig. 339.					
2a	Crystal growth: Crystal growth of $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$ was reported by MYL'NIKOVA.					60M2
3	Crystal structure: $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$ has the structure of perovskite type. Fig. 339. $Z = 64$ (molecular unit: $\text{Pb}_2\text{MgWO}_6$ ).					62Z1
4	Lattice distortion associated with the phase transition. Thermal expansion: Fig. 340.					62Z1
5a	Dielectric constants: Fig. 341, 342, 343. $d\Theta_a/dp = -5.84 \cdot 10^8 \text{ }^\circ\text{K N}^{-1}\text{m}^2$ .					
6	Specific heat: Fig. 344. Transition heat ( $\text{II} \rightarrow \text{I}$ ): $4Q_m = 276 \text{ cal mol}^{-1}$ .					66S28
8a	Elastic compliance: Fig. 345. Ultrasound absorption: Fig. 346, 347.					

Nr. 1B2-ii  $\text{Pb}(\text{Cd}_{1/2}\text{W}_{1/2})\text{O}_3$ 

1a	Synthesis of $\text{Pb}(\text{Cd}_{1/2}\text{W}_{1/2})\text{O}_3$ was reported by BELYAEV et al. in 1963.					63B3
b	phase	II	I			
	state	(A)	P			
	crystal system	monoclinic	cubic			65F4
	$\Theta$	400	°C			
	$a = (4.156 \pm 0.002) \text{ \AA}$ , $b = (4.074 \pm 0.002) \text{ \AA}$ , $\beta = 91^\circ 9' \pm 5'$ at RT. ROGINSKAYA and VENEVTSEV reported that another transition exists at 120 °C, in addition to the transition at 400 °C.					65R4
3	Crystal structure: Superstructure lines, indicating ordered location of the octahedral voids of the perovskite lattice, were observed.					65F4
4	Lattice distortion: Fig. 348, 349.					
5a	Dielectric constant: Fig. 350.					

Nr. 1B2-iii  $\text{Pb}(\text{Mn}_{1/2}\text{W}_{1/2})\text{O}_3$ 

1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{W}_{1/2})\text{O}_3$ was reported by VENEVTSEV et al.				64V3
b	phase	II	I		
	state	(A), $P_{\text{magn}}$	$P, P_{\text{magn}}$		
	crystal system	monoclinic	cubic		
	$\Theta$	423	$^{\circ}\text{K}$		
		$a = 4.063 \text{ \AA}$	$b = 4.033 \text{ \AA}$ , $\beta = 90^{\circ} 12'$ at RT.		
5a	Dielectric constant: Fig. 351.				65R5
10	Electrical conductivity: $\sigma = 8 \cdot 10^{-8} \Omega^{-1} \text{ m}^{-1}$ .				65R5
11	Magnetic susceptibility: see Fig. 351.				65R5

Nr. 1B2-iv  $\text{Pb}(\text{Co}_{1/2}\text{W}_{1/2})\text{O}_3$ 

1a	Antiferro- and ferroelectric properties in $\text{Pb}(\text{Co}_{1/2}\text{W}_{1/2})\text{O}_3$ were discovered by FILIP'EV et al.				63F1
b	phase	IV	III	II	I
	state	$F, F_{\text{magn}}$ (weak)	$F, P_{\text{magn}}$	$A, P_{\text{magn}}$	$P, P_{\text{magn}}$
	crystal system			orthorhombic	cubic
	$\Theta$	9 <sup>a)</sup>	83 ... 103	293 <sup>b)</sup> 305	$^{\circ}\text{K}$
		$a = 4.008 \text{ \AA}$ at 298 $^{\circ}\text{K}$ .			
2a	Crystal growth: Flux method with $\text{PbO}$ .				65B8
3	Crystal structure: A superstructure was observed which was completely explained by alternation of the population of the oxygen octahedra by $\text{Co}^{2+}$ and $\text{W}^{6+}$ cations along the three directions. The real elementary lattice is a cubic face centered one with the parameter $A = 2a$ for phase I and with the parameters $A = 2 \cos(\beta/2)$ , $B = 2b$ , and $C = 2a \sin(\beta/2)$ for II, where $a$ , $b$ and $\beta$ are the parameters of the perovskite sub-lattice.				64F4
4	phase	lattice parameters			
	I	$A = 8.017 \text{ \AA}$ at 298 $^{\circ}\text{K}$			
	II	$A = 5.669 \text{ \AA}$ , $B = 7.956 \text{ \AA}$ , $C = 5.689 \text{ \AA}$ at 258 $^{\circ}\text{K}$			
	Lattice distortion: Fig. 352.				64F4
5a	Dielectric constant: Fig. 353, 354, 355.				
c	Polarization: Fig. 356.				
11	Magnetic susceptibility and magnetization: Fig. 357, 358.				

Nr. 1B2-v  $\text{Pb}(\text{Mn}_{1/2}\text{Re}_{1/2})\text{O}_3$ 

1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{Re}_{1/2})\text{O}_3$ was reported by VENEVTSEV et al.				64V3
b	phase	III	II	I	
	state	(A), $F_{\text{magn}}$	(A), $P_{\text{magn}}$	$P, P_{\text{magn}}$	
	crystal system		monoclinic	cubic	
	$\Theta$	103	393	$^{\circ}\text{K}$	
		$a = 4.043 \text{ \AA}$	$b = 4.012 \text{ \AA}$	$\beta = 90^{\circ} 33'$ at RT.	
3	Crystal structure: Ordered perovskite.				65R5

4  
 10  
 11  
 Nr. 1  
 1a  
 b  
 -  
 -  
 3  
 5a  
 c  
 Nr. 1  
 1a  
 -  
 Nr. 1  
 1a  
 b  
 -  
 -  
 2a  
 3  
 5a  
 9a  
 11  
 12b  
 c

4	Lattice distortion: Fig. 359.	65R5																								
10	Electrical conductivity: $\sigma = 1 \cdot 10^{-1} \Omega^{-1} m^{-1}$ .	65R5																								
11	Magnetic susceptibility and magnetic moment: Fig. 360. The linear temperature dependence of $\chi_{\text{magn}}^1$ with a positive value of $\Theta_{\text{pmagn}} = 85^\circ\text{K}$ , and the appearing of the spontaneous moment at $103^\circ\text{K}$ , may indicate the presence of ferromagnetic properties in this compound, which is in agreement with the positive sign of the indirect exchange interaction proposed by GOODENOUGH for $\text{Mn}^{2+}$ and $\text{Re}^{8+}$ ions. However, the magnitudes of the calculated theoretical spontaneous moments agree with the experimental values only on the assumption of an anti-ferromagnetic interaction between ions distributed in an ordered fashion over the octahedral vacancies.	65R5																								
<b>Nr. 1B3-i <math>\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3</math></b>																										
1a b	Ferroelectricity in $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$ was discovered by SMOLENSKII et al. in 1959.  <table border="1"> <tr> <td>phase</td> <td>II</td> <td>I</td> </tr> <tr> <td>state</td> <td>F</td> <td>P</td> </tr> <tr> <td>crystal system</td> <td>tetragonal*) (possibly)</td> <td>cubic</td> </tr> <tr> <td><math>\Theta</math></td> <td>90</td> <td><math>^\circ\text{C}</math></td> </tr> <tr> <td><math>a = (4.074 \pm 0.001) \text{\AA}</math>, <math>c = (4.083 \pm 0.001) \text{\AA}</math> at RT.*</td> <td colspan="2"></td> </tr> </table>	phase	II	I	state	F	P	crystal system	tetragonal*) (possibly)	cubic	$\Theta$	90	$^\circ\text{C}$	$a = (4.074 \pm 0.001) \text{\AA}$ , $c = (4.083 \pm 0.001) \text{\AA}$ at RT.*			59S9 59S9 *)60I3									
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3	Crystal structure: In the powder patterns, additional to the principal lines of the perovskite structure, superstructural lines were observed indicating a doubling of the lattice period.	59I3																								
5a c	Dielectric constant: Fig. 361. Spontaneous polarization: $P_s \approx 3.6 \cdot 10^{-2} \text{ cm}^{-2}$ at $18^\circ\text{C}$ .	59S9																								
<b>Nr. 1B3-ii <math>\text{Pb}(\text{Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3</math></b>																										
1a	A synthesis of $\text{Pb}(\text{Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3$ with perovskite structure was reported by VENEV-TSEV et al.	64V3																								
<b>Nr. 1B3-iii <math>\text{Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3</math></b>																										
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phase	III	II	I																							
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$a = 4.014 \text{\AA}$ , $\alpha = 89.92^\circ$ at RT.			62B10																							
2a	Crystal growth: Flux method with $\text{PbO}$ .	62B7																								
3	Crystal structure: Disordered perovskite; X-ray studies have not shown any ionic ordering in the octahedral sites of perovskite structure. The magnetic peak was found in the neutron diffraction experiments at $78^\circ\text{K}$ . The effective magnetic moment of the $\text{Fe}^{3+}$ ion was found to be $(0.80 \pm 0.16) \mu_B$ at $78^\circ\text{K}$ from the calculation of the intensity of the (111) reflection, which is about 90% of the magnetic moment at $0^\circ\text{K}$ . Fig. 362.	64S8 65D6																								
5a	Dielectric constant: Fig. 363.																									
9a	Optical absorption: Fig. 364.																									
11	Magnetic susceptibility: Fig. 365. $\mu_{\text{eff}} = 5.4 \mu_B$ .	62B7																								
12b c	ESR: Fig. 366. Mössbauer effect: Fig. 367, 368. The quadrupole splitting $\Delta E_{\text{qu}} = (0.37 \pm 0.02) \text{ mm sec}^{-1}$ , the isomer shift $\delta = (0.52 \pm 0.02) \text{ mm sec}^{-1}$ , corresponding to trivalent iron (at $20^\circ\text{C}$ ).	66S22																								

Figuren S. 283

II 1 Oxide des Perowskit-Typs

Nr. 1B3-iv  $\text{Pb}(\text{Co}_{1/2}\text{Nb}_{1/2})\text{O}_3$

- 1a | A synthesis of  $\text{Pb}(\text{Co}_{1/2}\text{Nb}_{1/2})\text{O}_3$  with perovskite structure was reported by VENEV-TSEV et al.  
b | Informations on the dielectric and magnetic properties are available:

64V3  
65R5

Nr. 1B3-v  $\text{Pb}(\text{Ni}_{1/2}\text{Nb}_{1/2})\text{O}_3$

- 1a |  $\text{Pb}(\text{Ni}_{1/2}\text{Nb}_{1/2})\text{O}_3$  with perovskite structure was synthesized by the addition of 5 mol %  $\text{BaO}$ .

65S17

Nr. 1B3-vi  $\text{Pb}(\text{In}_{1/2}\text{Nb}_{1/2})\text{O}_3$

- 1a | Dielectric anomaly in  $\text{Pb}(\text{In}_{1/2}\text{Nb}_{1/2})\text{O}_3$  was found by KUPIRIYANOV and FESENKO in 1965.

b	phase	II	I	65K9
	state	(F)	P	
	crystal system	monoclinic (possibly)	cubic	65K9
	$\Theta$	90	°C	

$a = 4.11 \text{ \AA}$  at RT.

- 5a | Dielectric constant: Fig. 369.

Nr. 1B3-vii  $\text{Pb}(\text{Yb}_{1/2}\text{Nb}_{1/2})\text{O}_3$

- 1a | Antiferroelectric properties in  $\text{Pb}(\text{Yb}_{1/2}\text{Nb}_{1/2})\text{O}_3$  were reported by FILIP'EV et al. in 1963.

b	phase	II	I	63F1
	state	AF	P	
	crystal system	monoclinic	cubic	65K9
	$\Theta$	300, 310 <sup>a)</sup>	°C	

$a = 4.168 \text{ \AA}$ ,  $b = 4.107 \text{ \AA}$ ,  $\beta = 90^\circ 27'$  at RT<sup>a)</sup>.

- 3 | Crystal structure: Superstructure lines, corresponding to ordering of  $\text{Yb}^{3+}$  and  $\text{Nb}^{5+}$  ions were found.

- 4 | Lattice distortion: Fig. 370.  
Thermal expansion: Fig. 371.

- 5a | Dielectric constant: Fig. 372.

Nr. 1B3-viii  $\text{Pb}(\text{Ho}_{1/2}\text{Nb}_{1/2})\text{O}_3$

- 1a | Dielectric anomaly in  $\text{Pb}(\text{Ho}_{1/2}\text{Nb}_{1/2})\text{O}_3$  was found by KUPIRIYANOV and FESENKO.

b	phase	II	I	65K9
	state	(A)	P	
	crystal system	monoclinic	cubic	
	$\Theta$	240	°C	

$a = 4.160 \text{ \AA}$ ,  $b = 4.106 \text{ \AA}$ ,  $\beta = 90^\circ 30'$  at RT.

- 5a | Dielectric constant: Fig. 373.

Nr. 1B3-ix  $\text{Pb}(\text{Lu}_{1/2}\text{Nb}_{1/2})\text{O}_3$

- 1a | Dielectric anomaly in  $\text{Pb}(\text{Lu}_{1/2}\text{Nb}_{1/2})\text{O}_3$  was found by SMOLENSKII and AGRANOV-SKAYA in 1958.

58S3

1b	phase	II	I	
	state	(A)	P	
	crystal system	monoclinic	cubic	
	$\Theta$	270	°C	65K9
	$a = 4.152 \text{ \AA}$ , $b = 4.093 \text{ \AA}$ , $\beta = 90^\circ 30'$ at RT.			
4	Thermal expansion: Fig. 374.			
5a	Dielectric constant: Fig. 375.			

Nr. 1B3-x  $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$ 

1a b	Ferroelectricity in $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$ was discussed by SMOLENSKII et al. in 1959.	59S9		
	phase	II	I	
	state	F	P	59S9
	crystal system	tetragonal <sup>a)</sup> (possibly)	cubic	<sup>a)</sup> 59I3
	$\Theta$	26	°C	
	$a = (4.072 \pm 0.001) \text{ \AA}$ , $c = (4.072 \pm 0.001) \text{ \AA}$ at RT <sup>a)</sup> .			
3	Crystal structure: The large number of superstructure lines and their great intensity in $\text{Pb}(\text{Sc}_{1/2}\text{Ta}_{1/2})\text{O}_3$ indicates that the degree of ordering of $\text{Sc}^{3+}$ and $\text{Ta}^{5+}$ ions is greater than in $\text{Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$ . See 1B3-i-3.			59I3
5a	Dielectric constant: Fig. 376.			

Nr. 1B3-xi  $\text{Pb}(\text{Mn}_{1/2}\text{Ta}_{1/2})\text{O}_3$ 

1a	$\text{Pb}(\text{Mn}_{1/2}\text{Ta}_{1/2})\text{O}_3$ with perovskite structure was synthesized by the addition of 5 mol% $\text{SrO}$ .	65S17
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Nr. 1B3-xii  $\text{Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$ 

1a b	Ferroelectricity in $\text{Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$ was discovered by SMOLENSKII et al. in 1959.	59S7		
	phase	III	II	I
	state	F, A <sub>magn</sub>	F, P <sub>magn</sub>	P, P <sub>magn</sub>
	crystal system	rhombohedral	rhombohedral <sup>a)</sup>	cubic
	space group			Pm3m-O <sub>h</sub>
	$\Theta$	143, 133 <sup>a)</sup>	243, 233 <sup>a)</sup>	°K
	$P_s \parallel [111]$ (probably).			
	$a = (4.007 \pm 0.001) \text{ \AA}$ at RT.			
	black (dark orange for thin samples).			
2a	Crystal growth: Flux method with $\text{PbO}$ . When the soak temperature is higher than 1200 °C, crystals are obtained having both pyrochloride and perovskite structure.	68N1		
3	Crystal structure: Disordered perovskite.	65S17		
4	phase	lattice constants		
	I	$a = (4.007 \pm 0.001) \text{ \AA}$ at RT.		
	II	$a = (4.006 \pm 0.001) \text{ \AA}$ at 90 °K $\alpha = 89.89^\circ \pm 0.02^\circ$		
5a c	Dielectric constant: Fig. 377, 378. Spontaneous polarization: Fig. 379.			
11	Magnetic susceptibility: Fig. 380. $\mu_{\text{eff}} = 5.92 \mu_B$ ; $\Theta_{\text{p,magn}} = -370$ °K.			68N1

Figuren S. 285

II 1 Oxide des Perowskit-Typs

Nr. 1B3-xiii  $\text{Pb}(\text{Co}_{1/2}\text{Ta}_{1/2})\text{O}_3$

1a A synthesis of  $\text{Pb}(\text{Co}_{1/2}\text{Ta}_{1/2})\text{O}_3$  with perovskite structure was reported by SHVORNEVA and VENEVTSOV. The compound was stabilized by the addition of 1 mol%  $\text{La}_2\text{O}_3$ . 65S17

Nr. 1B3-xiv  $\text{Pb}(\text{Yb}_{1/2}\text{Ta}_{1/2})\text{O}_3$

1a	Dielectric anomaly in $\text{Pb}(\text{Yb}_{1/2}\text{Ta}_{1/2})\text{O}_3$ was reported by ISUPOV and KRAKIN in 1964.			64I6
b	phase	II	I	
	state	(A)	F	
	crystal system	monoclinic	cubic	
	$\Theta$	280, 285 <sup>a)</sup> °C		
	$a$	$a = 4.154 \text{ \AA}$ , $b = 4.108 \text{ \AA}$ , $\beta = 90^\circ 30'$ at RT.		

4 Thermal expansion: Fig. 381.

5a Dielectric constant: Fig. 382.

Nr. 1B3-xv  $\text{Pb}(\text{Lu}_{1/2}\text{Ta}_{1/2})\text{O}_3$

1a	Dielectric anomaly in $\text{Pb}(\text{Lu}_{1/2}\text{Ta}_{1/2})\text{O}_3$ was found by SMOLENSKII and AGRANOV-SKAYA in 1958.			58S3
b	phase	II	I	
	state	(A)	P	
	crystal system	monoclinic	cubic	
	$\Theta$	280 °C		
	$a$	$a = 4.153 \text{ \AA}$ , $b = 4.107 \text{ \AA}$ , $\beta = 90^\circ 30'$ at RT.		
4	Lattice distortion: Fig. 383. Thermal expansion: Fig. 384.			
5	Dielectric constant: Fig. 385.			

Nr. 1B3-xvi  $\text{Pb}(\text{Fe}_{1/2}\text{W}_{1/2})\text{O}_3$

1a	A synthesis of $\text{Pb}(\text{Fe}_{1/2}\text{W}_{1/2})\text{O}_3$ with perovskite structure was reported by VENEVTSOV et al.			64V3
b	The magnetic measurements confirmed the presence of the spinel phase in a sample of this composition.			65R5

Nr. 1B3-xvii  $\text{Pb}(\text{Li}_{1/4}\text{Nb}_{1/4}\text{W}_{1/2})\text{O}_3$  and sister crystals

1a	Following composite perovskite compounds containing Pb were synthesized: $\text{Pb}(\text{Li}_{1/4}\text{Nb}_{1/4}\text{W}_{1/2})\text{O}_3$ $\text{Pb}(\text{Zn}_{1/4}\text{Mn}_{1/4}\text{Nb}_{1/2})\text{O}_3$ $\text{Pb}(\text{Co}_{1/4}\text{Mn}_{1/4}\text{W}_{1/2})\text{O}_3$ $\text{Pb}(\text{Mg}_{1/4}\text{Mn}_{1/4}\text{Nb}_{1/2})\text{O}_3$ $\text{Pb}(\text{Cd}_{1/4}\text{Mn}_{1/4}\text{Nb}_{1/2})\text{O}_3$ $\text{Pb}(\text{Ni}_{1/4}\text{Mn}_{1/4}\text{W}_{1/2})\text{O}_3$ $\text{Pb}(\text{Co}_{1/4}\text{Mn}_{1/4}\text{Nb}_{1/2})\text{O}_3$ $\text{Pb}(\text{Mg}_{1/4}\text{Mn}_{1/4}\text{Ta}_{1/2})\text{O}_3$ $\text{Pb}(\text{Cd}_{1/4}\text{Mn}_{1/4}\text{W}_{1/2})\text{O}_3$ $\text{Pb}(\text{Ni}_{1/4}\text{Mn}_{1/4}\text{Nb}_{1/2})\text{O}_3$ $\text{Pb}(\text{Mg}_{1/4}\text{Mn}_{1/4}\text{W}_{1/2})\text{O}_3$ $\text{Pb}(\text{Sc}_{1/4}\text{Cr}_{1/4}\text{Nb}_{1/2})\text{O}_3$			
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Nr. 1B4-i  $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$

1a	Ferroelectricity in $\text{Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$ was discovered by SMOLENSKII and AGRANOV-SKAYA in 1958.			58S3, 59S6
b	phase	II	I	
	state	F	P	
	crystal system		cubic	
	space group		Pm3m-O <sub>h</sub>	
	$\Theta$	265 <sup>a)</sup> °K		
	$\rho$	$\rho = 8.12 \cdot 10^3 \text{ kg m}^{-3}$ , $a = 4.04 \text{ \AA}$ at RT. Transparent, pale yellow.		
				61B5, 60S7 a) 67B9 67B18

2a	Crystal growth: Flux method (using PbO). Kyropoulos method.	59M5 67B18
3	Crystal structure: Disordered perovskite.	61B5
4	Thermal expansion: Fig. 386.	
5a	Dielectric constant: Fig. 387, 388, 389.	
b	Nonlinear dielectric properties: $E = [(T - \Theta_p)(\epsilon_0 C)^{-1}] P + \xi P^3 + \zeta P^5 + \dots$ , where $\Theta_p = 265$ °K, $C = (3.7 \pm 1.0) \cdot 10^5$ °K, and $\xi \cong 5.6 \cdot 10^8$ V m <sup>5</sup> C <sup>-3</sup> .	67B9
c	Spontaneous polarization and coercive field: Fig. 390.	
7a	Piezoelectricity: Fig. 391.	
9a	Refractive index: $n = 2.56$ for 6328 Å at 299 °K. Birefringence: It was found that the crystals $Pb(Mg_{1/3}Nb_{2/3})O_3$ behave like optically isotropic crystals. An applied electric field causes double refraction. Fig. 392.	67B9
e	Quadratic electrooptic effect: $M_{11} - M_{12} = +0.015$ m <sup>4</sup> C <sup>-2</sup> , $M_{44} = +0.008$ m <sup>4</sup> C <sup>-2</sup> for 6328 Å at 299 °K.	67B9
14a	Domain structure: Clear domains were observed only in very thin wafers (e. g., $20 \cdot 10^{-6}$ m).	61B5

Nr. 1B4-ii  $Pb(Zn_{1/3}Nb_{2/3})O_3$ 

1a	Ferroelectric $Pb(Zn_{1/3}Nb_{2/3})O_3$ crystal was synthesized by BOKOV and MYL'NIKOVA in 1960.	60B7
b	phase                    II                    I state                    F                    P crystal system            cubic $\Theta$ 140                    °C	60B7
	$a = 4.04$ Å at RT. light yellow.	
2a	Crystal growth: Flux method with PbO. The crystals were separated from the matrix solution by washing in acetic acid at RT for a long time.	60B7
5a	Dielectric constant: Fig. 393.	

Nr. 1B4-iii  $Pb(Cd_{1/3}Nb_{2/3})O_3$ 

1b	Dielectric anomaly in $Pb(Cd_{1/3}Nb_{2/3})O_3$ was reported by VENEVTSEV et al. in 1966.	65T5, 66V5
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Nr. 1B4-iv  $Pb(Co_{1/3}Nb_{2/3})O_3$ 

1a	Ferroelectricity in $Pb(Co_{1/3}Nb_{2/3})O_3$ was found by BOKOV and MYL'NIKOVA in 1960.	60B7
b	phase                    II                    I state                    F                    P crystal system            cubic space group              Pm3m-O <sub>h</sub> $\Theta$ -98                    °C	60B7
	$a = 4.04$ Å at RT. brown.	
2a	Crystal growth: Flux method with PbO.	60B7
5a	Dielectric constant: Fig. 394.	

Nr. 1B4-v  $\text{Pb}(\text{Ni}_{1/3}\text{Nb}_{2/3})\text{O}_3$ 

1a Ferroelectricity in  $\text{Pb}(\text{Ni}_{1/3}\text{Nb}_{2/3})\text{O}_3$  was discovered by SMOLENSKII and AGRANOV-SKAYA in 1958.

b	phase	II	I
	state	F	P
	crystal system		cubic
	space group		Pm3m-O <sub>h</sub> <sup>1</sup>
	$\Theta$	153	°K

$a = 4.03 \text{ \AA}$  at RT.  $\rho = 8.55 \cdot 10^3 \text{ kg m}^{-3}$ . yellowish green.

58S3, 59S6

61B5, 60S7

59M5

59M5

59M5

61B5

2a Crystal growth: Flux method with PbO.

3 Crystal structure: Disordered perovskite.

4 Thermal expansion: Fig. 395.

5a Dielectric constant: Fig. 396, 397, 398.

9a Birefringence: Fig. 399.

Nr. 1B4-vi  $\text{Pb}(\text{Mg}_{1/3}\text{Ta}_{2/3})\text{O}_3$ 

1a Ferroelectricity in  $\text{Pb}(\text{Mg}_{1/3}\text{Ta}_{2/3})\text{O}_3$  was found by BOKOV and MYL'NIKOVA in 1960.

b	phase	II	I
	state	F	P
	crystal system		cubic
	space group		Pm3m-O <sub>h</sub> <sup>1</sup>
	$\Theta$	-98	°C

$a = 4.02 \text{ \AA}$  at RT.  
light yellow.

60B7

60B7

60B7

60B7

2a Crystal growth: Flux method with PbO.

3 Crystal structure: Disordered perovskite.

5a Dielectric constant: Fig. 400.

Nr. 1B4-vii  $\text{Pb}(\text{Co}_{1/3}\text{Ta}_{2/3})\text{O}_3$ 

1a Ferroelectricity in  $\text{Pb}(\text{Co}_{1/3}\text{Ta}_{2/3})\text{O}_3$  was found by BOKOV and MYL'NIKOVA in 1960.

b	phase	II	I
	state	F	P
	crystal system		cubic
	space group		Pm3m-O <sub>h</sub> <sup>1</sup>
	$\Theta$	-140	°C

$a = 4.01 \text{ \AA}$  at RT.  
brown.

60B7

60B7

60B7

60B7

2a Crystal growth: Flux method with PbO.

3 Crystal structure: Disordered perovskite.

5a Dielectric constant: Fig. 401.

Nr.

1a  
b

2a

3

5a

Nr.

1a

b

5a

10

11

Nr.

1a

b

2a

5a

11

12b

1C

Nr.

1b

5a

6a

7a

Nr. 1B4-viii $\text{Pb}(\text{Ni}_{1/3}\text{Ta}_{2/3})\text{O}_3$								
1a	Ferroelectricity in $\text{Pb}(\text{Ni}_{1/3}\text{Ta}_{2/3})\text{O}_3$ was found by BOKOV and MYL'NIKOVA in 1960.							
b	phase	II	I					
	state	F	P					
	crystal system		cubic					
	space group		Pm3m-O <sub>h</sub>					
	$\Theta$	—180	°C					
	$a = 4.01 \text{ \AA}$ at RT. green.							
2a	Crystal growth: Flux method.							
3	Crystal structure: Disordered perovskite.							
5a	Dielectric constant: Fig. 402.							
Nr. 1B5-i $\text{Pb}(\text{Mn}_{2/3}\text{W}_{1/3})\text{O}_3$								
1a	Dielectric and magnetic anomalies in $\text{Pb}(\text{Mn}_{2/3}\text{W}_{1/3})\text{O}_3$ were reported by ROGINSKAYA et al. in 1965.							
b	phase	III	II	I				
	state	(A), (A <sub>magn</sub> )	(A), P <sub>magn</sub>	P, P <sub>magn</sub>				
	crystal system		monoclinic	cubic				
	$\Theta$	203	473	°K				
	$a = c = 4.098 \text{ \AA}$ , $b = 4.014 \text{ \AA}$ , $\beta = 90^\circ 23'$ at RT.							
5a	Dielectric constant: Fig. 403.							
10	$\sigma = 2 \cdot 10^{11} \Omega^{-1} \text{ m}^{-1}$ .							
11	Magnetic susceptibility: see Fig. 403. $\Theta_{p\text{magn}} = -75 \text{ }^\circ\text{K}$ .							
Nr. 1B5-ii $\text{Pb}(\text{Fe}_{2/3}\text{W}_{1/3})\text{O}_3$								
1a	Ferroelectricity in $\text{Pb}(\text{Fe}_{2/3}\text{W}_{1/3})\text{O}_3$ was discovered by SMOLENSKII et al. in 1959.							
b	phase	III	II	I				
	state	F, A <sub>magn</sub>	P, A <sub>magn</sub>	P, P <sub>magn</sub>				
	crystal system		cubic	cubic				
	$\Theta$	178	363	°K				
	$a = 4.02 \text{ \AA}$ at RT.							
2a	Flux method (PbO).							
5a	Dielectric constant: Fig. 404.							
11	Magnetic susceptibility: see Fig. 404. Magnetization is a linear function of the magnetic field intensity up to 8000 Oe. Effective magnetic moment: $4.2 \mu_B$ .							
12b	ESR: Fig. 405.							
1C Solid solutions with perovskite-type oxides as end members								
Nr. 1C-a1 $\text{NaNbO}_3\text{-KNbO}_3$								
1b	Phase diagram: Fig. 406, 407, 408. Lattice parameters: Fig. 409.							
5a	Dielectric constant: Fig. 410; see Tab. 60. Polarization and coercive field: Fig. 411.							
6a	Transition energy: Tab. 59.							
7a	Electromechanical properties: Fig. 412 ... 417; Tab. 60.							

Tab. 59.  $(Na_{1-x}K_x)NbO_3$ . Transition energy  $\Delta Q_m$ . [54SJ]

$x$	Lower phase change	Upper phase change
1.00 ( $KNbO_3$ )	85 cal/mole	190 cal/mole
0.10	20 cal/mole	60 cal/mole
0 ( $NaNbO_3$ )	—	50 cal/mole

Tab. 60.  $(Na_{0.5}K_{0.5})NbO_3$  (ceramics). Electric and electromechanical constants. [59E7]

Dielectric constant (100 kHz)	290
Dissipation factor (100 kHz)	$\approx 4.0\%$
Specific resistivity $\rho$	$10^{10} \Omega m$
Density $\rho$	$4.25 \cdot 10^3 \text{ kg m}^{-3}$
Poisson's ratio (assumed)	0.27
Coupling factor $k_p$	$0.34 \dots 0.39$
Frequency constant $f_R$	1.67 kHz m
Mechanical $Q_{\text{mech}}$ (radial)	130
Young's modulus $E$	$1.04 \cdot 10^{11} \text{ N m}^{-2}$
Piezoelectric constant $-d_{31}$	$32 \cdot 10^{-12} \text{ C N}^{-1}$
Piezoelectric constant $-g_{31}$	$12.6 \cdot 10^{-8} \text{ m}^2 \text{ C}^{-1}$
Piezoelectric constant $d_{33}^*$	$80 \cdot 10^{-12} \text{ C N}^{-1}$
Piezoelectric constant $g_{33}^*$	$31.5 \cdot 10^{-8} \text{ m}^2 \text{ C}^{-1}$
Coupling factor $k_{33}^*$	0.51

Nr. 1C-a2  $NaNbO_3$ - $NaTaO_3$ 

- 1b | Phase diagram: Fig. 418.  
 Lattice parameters: Fig. 419.  
 4 | Thermal expansion: Fig. 420.  
 5a | Dielectric constant: Fig. 421.  
 9a | Birefringence: Fig. 422.

Nr. 1C-a3  $NaNbO_3$ - $NaSbO_3$ 

- 1a | Curie temperature: Fig. 423.

Nr. 1C-a4  $KNbO_3$ - $KTaO_3$ 

- 1 | Phase diagram: Fig. 424, 425.  
 5a | Dielectric properties: Fig. 426, 427.  
 $\Theta_f$ : see Tab. 61.  
 6 | Thermal properties: Fig. 428; Tab. 61.  
 9 | See 1C-a5 for optical properties of  $K(Ta_{0.35}Nb_{0.65})O_3$  (KTN).

Tab. 61.  $K(Nb_{1-x}Ta_x)O_3$ .  $L$ : latent heat,  $\Theta_f$ : Curie point,  $A$ : constant in the formula for free energy =  $A(T - \Theta_p)P^2 + \dots$ ,  $P_{\text{calc}}$ :  $P_s$  calculated for  $T = \Theta_f$ . [59H1]

$x$	$L$ cal mol $^{-1}$	$\Theta_f$ $^{\circ}\text{K}$	$A$ $10^5 \text{ }^{\circ}\text{K}^{-1}$	$P_{\text{calc}}$ $10^{-8} \text{ C m}^{-2}$
0	110 $\pm$ 10	679	2.6	27
0.06	46 $\pm$ 4	656	2.7	17.7
0.12	10 $\pm$ 2	623	2.85	7.9
0.18	4.0 $\pm$ 2	591	3.05	5.1

Nr. 1C-a5  $K(Ta_{0.35}Nb_{0.65})O_3$  (KTN)

For general properties of  $KNbO_3$ - $KTaO_3$  see 1C-a4.

- 9b | Electroreflectance: Fig. 429.  
 d | Faraday rotation: Fig. 430. See also Tab. 44.

Nr. 1C-a6  $CaTiO_3$ - $SrTiO_3$ 

- 1b | Phase diagram: Fig. 431, 432, 433.  
 Lattice parameters: Fig. 434.  
 5a | Dielectric constant: Fig. 435, 436.  
 c | Spontaneous polarization: Fig. 437.

Nr. 1C-a7  $CaTiO_3$ - $BaTiO_3$ 

- 1b | Phase diagram: Fig. 438, 439, 440.  
 Lattice parameters: Fig. 441.  
 5a | Dielectric constant: Fig. 442, 443.  
 6b | Thermal conductivity: Fig. 444.  
 7a | Electromechanical property: Tab. 62. See Fig. 183 and Tab. 40.

\* Estimated values.

Tab. 62.  $(\text{Ba}_{1-x}\text{Ca}_x)\text{TiO}_3$  (ceramics, pure  $\text{BaTiO}_3$  base).  $d_{31}$  and  $d_{33}$  at RT. [57B4]

$x$	$\rho$ $10^3 \text{ kg m}^{-3}$	$\rho_x$ $10^3 \text{ kg m}^{-3}$	$d_{31}$ $10^{-12} \text{ CN}^{-1}$	$d_{33}$ $10^{-12} \text{ CN}^{-1}$	$-d_{33}/d_{31}$	Porosity $(1 - (\rho/\rho_x))$
0	5.85	6.017	-97.5	229	2.35	0.028
0.05	5.70	5.85	-66.6	167	2.51	0.026
0.07	5.68	5.80	-58.0	150	2.58	0.021
0.09	5.65	5.74	-52.1	139	2.67	0.016
0.12	5.55	5.66	-43.4	124.5	2.88	0.019

**Nr. 1C-a8  $\text{CaTiO}_3\text{-PbTiO}_3$** 1b | Curie temperature: Fig. 445.  
Lattice parameter: Fig. 446.**Nr. 1C-a9  $\text{SrTiO}_3\text{-BaTiO}_3$** 1b | Phase diagram: Fig. 447 ... 450.  
Lattice parameter: Fig. 451; see Fig. 448.5a | Dielectric constant: Fig. 452.  
Microwave dielectric loss: Tab. 63.

6a | Specific heat: Fig. 453.

10b | Conductivity associated with doping: Fig. 454, 455, 456.

Tab. 63.  $(\text{Ba}_{1-x}\text{Sr}_x)\text{TiO}_3$ . Dielectric loss:  $\alpha, \beta, \gamma$  at 20 GHz. [62R4].  $(T - \Theta_p) \tan \delta = \alpha + \beta T + \gamma T^2$ .

Sample		Heat treatment	Grain size $\mu$	$\Theta_p$ $^\circ\text{K}$	$\alpha$ $^\circ\text{K}$	$\beta \cdot 10^4$	$\gamma \cdot 10^6$ $(^\circ\text{K})^{-1}$
Polycrystalline	$\text{SrTiO}_3$	Hot pressed and fired in air at 900 °C for 10 h	1	37	0.33	7.7	4.3
		Refired at 1200 °C in air for 10 h	3	37	0.26	5.5	4.7
		Refired at 1400 °C in air for 10 h	15	37	0.17	4.4	4.2
		Refired at 1500 °C in $\text{O}_2$ for 6 h	30	37	0.08	4.5	3.7
	$\text{Ba}_{0.2}\text{Sr}_{0.8}\text{TiO}_3$	Hot pressed and fired in $\text{O}_2$ at 1500 °C for 10 h	30	105	0.6	9	2.5
	$\text{Ba}_{0.5}\text{Sr}_{0.5}\text{TiO}_3$	Hot pressed and fired in $\text{O}_2$ at 1500 °C for 10 h	30	218	2.0	(9) <sup>a)</sup>	(2.5)
	$\text{Ba}_{0.7}\text{Sr}_{0.3}\text{TiO}_3$	Ceramic fired to 1375 °C in air for 1 h	8	280	2.2	(9)	(2.5)
	$\text{Ba}_{0.8}\text{Sr}_{0.2}\text{TiO}_3$	Ceramic fired to 1300 °C in air for 1 h	8	324	1.6	(9)	(2.5)
Single crystal	$\text{SrTiO}_3$	None	$\infty$	37	0	6.53	2.54
	$\text{SrTiO}_3 + 0.1\% \text{Gd}^{3+}$	None	$\infty$	37	0.033	(6.53)	(2.54)
	$\text{SrTiO}_3 + 0.03\% \text{Fe}^{3+}$	None	$\infty$	37	0.043	(6.53)	(2.54)

**Nr. 1C-a10  $\text{SrTiO}_3\text{-PbTiO}_3$** 1b | Curie temperature: Fig. 457.  
Lattice parameter: Fig. 458.5a | Dielectric constant: Fig. 459.  
Curie constant: Fig. 460.

6a | Transition heat: Fig. 461.

**Nr. 1C-a11  $\text{BaTiO}_3\text{-PbTiO}_3$** 1b | Phase diagram: Fig. 462.  
Lattice parameter: Fig. 463.

5a | Dielectric constant: Fig. 464.

6a | Specific heat: Fig. 465.  
Transition heat: Fig. 466.

7 | Electromechanical properties: see 1A-8.

16 | Radiation damage: Fig. 467.

<sup>a)</sup> Values in parentheses indicate that these values were assumed in order to determine  $\alpha$ .

Nr. 1C-a12 $\text{CaZrO}_3\text{-BaZrO}_3$	1b   Lattice parameter: Fig. 468.
Nr. 1C-a13 $\text{CaZrO}_3\text{-PbZrO}_3$	1b   Phase diagram: Fig. 469. 4   Thermal expansion: Fig. 470. 5a   Dielectric constant: Fig. 471.
Nr. 1C-a14 $\text{SrZrO}_3\text{-PbZrO}_3$	1b   Phase diagram: Fig. 472, 473. Lattice parameter: Fig. 474. 4   Thermal expansion: Fig. 475, 476, 477; Tab. 64. 5a   Dielectric constant: Fig. 478, 479. c   Polarization: Fig. 480. 6a   Specific heat: Fig. 481. Transition heat: Tab. 65.

Tab. 64.  $\text{PbZrO}_3$ ,  $(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$ , and  $(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$ .  $\Delta V/V$ .  $\Delta V$ : anomalous volume change at the transition point. [54S2]

Composition	$\Delta V/V [10^{-4}]$	
	Lowest phase	Intermediate phase
$\text{PbZrO}_3$	-41 at 230 °C	-
$(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$	-43 at 150 °C	+24 at 190 °C
$(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$	-30 at 210 °C	-20 at 230 °C

Tab. 65.  $\text{PbZrO}_3$ ,  $(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$ , and  $(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$ .  $\Delta Q_m$ . [52S2]

Composition	$\Delta Q_m [\text{cal mol}^{-1}]$	
	Lower transition	Upper transition
$\text{PbZrO}_3$	-	440
$(\text{Pb}_{0.925}\text{Ba}_{0.075})\text{ZrO}_3$	190	230
$(\text{Pb}_{0.95}\text{Sr}_{0.05})\text{ZrO}_3$	180	230

Nr. 1C-a15 $\text{BaZrO}_3\text{-PbZrO}_3$	1b   Phase diagram: Fig. 482. Lattice parameter: Fig. 483. 4   Thermal expansion: Fig. 484. 5a   Dielectric constant: Fig. 485 ... 488. c   Coercive field: Fig. 489. 8   Elastic properties: Fig. 490.
Nr. 1C-a16 $\text{CaHfO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 491. 5a   Dielectric constant: Fig. 492.
Nr. 1C-a17 $\text{SrHfO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 493. 5a   Dielectric constant: Fig. 494.
Nr. 1C-a18 $\text{BaHfO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 495.
Nr. 1C-a19 $\text{CaSnO}_3\text{-SrSnO}_3$	1b   Lattice parameter: Fig. 496.
Nr. 1C-a20 $\text{BaSnO}_3\text{-SrSnO}_3$	1b   Lattice parameter: see Fig. 496.
Nr. 1C-a21 $\text{BaSnO}_3\text{-PbO:SnO}_2$	1b   Phase diagram: Fig. 497. 5a   Dielectric constant: Fig. 498.
Nr. 1C-a22 $\text{CaTiO}_3\text{-CaZrO}_3$	1b   Lattice parameter: Fig. 499.

Nr. 1C-a23 $\text{BaTiO}_3\text{-BaZrO}_3$	1b	Phase diagram: Fig. 500. Lattice parameter: Fig. 501.			
	2a	Phase diagram: Fig. 502.			
	5a	Dielectric constant: Fig. 503.			
	8a	Elastic property: Fig. 504			
Nr. 1C-a24 $\text{BaTiO}_3\text{-BaHfO}_3$	1b	Phase diagram: Fig. 505. Lattice parameter: Fig. 506.			
	5a	Dielectric constant: Fig. 507.			
Nr. 1C-a25 $\text{BaTiO}_3\text{-BaSnO}_3$	1b	Phase diagram: Fig. 508. See also	59I2		
	2a	Phase diagram: Fig. 509.			
	4	Thermal expansion: Fig. 510.			
	5a	Dielectric constant: Fig. 511.			
Nr. 1C-a26 $\text{BaTiO}_3\text{-BaUO}_3$	1b	Lattice parameter: Fig. 512.			
Nr. 1C-a27 $\text{PbTiO}_3\text{-PbZrO}_3$ $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$ with $x = 0.5 \dots 0.6$ ; for electromechanical properties of these very important piezoelectric materials, see 1C-a28.	1a	Ferro- and antiferroelectric phase transitions in the $\text{PbTiO}_3\text{-PbZrO}_3$ system were revealed in 1952 by SHIRANE, SUZUKI and TAKEDA.	52S6, 52S4, 52S3		
	b	Phase diagram at high temperature: Fig. 513. Phase diagram: Fig. 514, 515. Lattice parameter: Fig. 516, 517.			
	2	Flux method:	62I1, 64F6, 67F7		
	4	Lattice distortion: Fig. 518a, b, 519. Thermal expansion: Fig. 520, 521, 522.			
	5a	Dielectric constant: Fig. 523 $\dots$ 526.			
	c	Spontaneous polarization: Fig. 527. Critical field: Fig. 528.			
	6	Specific heat: Fig. 529, 530. Transition energy: Tab. 66.			
	7 8}	Electromechanical properties: see 1C-a28.			
	9	Birefringence: Fig. 531a, b, c.			
	16	Radiation damage: Fig. 532.			
Tab. 66. $\text{Pb}(\text{Zr}-\text{Ti})\text{O}_3$ . Transition energy and entropy. [53S1]. $x$ : atomic percent of $\text{PbTiO}_3$ ; $d\Theta/dx$ : shift of the transition temperature with $x$ ; $dS(d\Theta/dx)$ : it may be assumed that the free energy should decrease with the rate of $dS(d\Theta/dx)$ with increasing $x$ .					
Kind of the phase change	$\Theta$ °C	$\Delta Q_m$ cal mol $^{-1}$	$\Delta S_m$ cal mol $^{-1}$ K $^{-1}$	$d\Theta/dx$	$dS(d\Theta/dx)$
$A_\alpha \rightarrow P_\alpha$	230 $> T >$ 225	400	0.8	—	(-5.8)
$A_\alpha \rightarrow A_\beta$	225	110	0.22	-16	-3.5
$A_\beta \rightarrow P_\alpha$	230	290	0.58	-4	-2.3
$A_\alpha \rightarrow F_\alpha$	240	—	—	-19	—
$F_\alpha \rightarrow P_\alpha$	217	250	0.51	+1.0	+0.5
$A_\beta \rightarrow F_\alpha$	—	40	0.08	—	—

Nr. 1C-a28  $\text{Pb}(\text{Zr}_x\text{Ti}_{1-x})\text{O}_3$  ( $x = 0.5 \dots 0.6$ , lead zirconate-titanate)  
For general properties of  $\text{PbTiO}_3$ - $\text{PbZrO}_3$  see 1C-a27.

1a	JAFFE, ROTH, and MARZULLO discovered the excellent piezoelectric performances of $\text{Pb}(\text{Zr}-\text{Ti})\text{O}_3$ ceramics in 1954. PZT is the trade mark of this substance developed by Clevite Corporation, Cleveland, Ohio, USA.									54J1		
5a	Dielectric constants: Fig. 533 and Fig. 539, 540, 541, 543, 544.											
7)	Electromechanical properties (ceramics): Tab. 67; Fig. 534 ... 538; Tab. 68 ... 72; Fig. 539 ... 542; Tab. 73; Fig. 543 ... 554.											
8)	Electrical conductivity: see For breakdown, see									63G1, 61S14 59G2		
Tab. 67. $\text{Pb}(\text{Ti}_{1-x}\text{Zr}_x)\text{O}_3$ [ $x = 0.48 \dots 0.60$ ] (ceramics). Electromechanical constants at RT. [60B3]												
Zr/Ti atom ratio	$k_{31}$	$k_p$	$k_{15}$	$k_{33}$	$\kappa_{11}^T$	$\kappa_{11}^S$	$\kappa_{33}^T$	$\kappa_{33}^S$ obs	$\kappa_{33}^S$ calc			
48/52	0.170	0.289	0.408	0.435	663	551	666	540	537			
50/50	0.230	0.397	0.504	0.546	855	631	846	585	585			
52/48	0.313	0.529	0.694	0.670	1180	612	730	399	389			
54/46	0.280	0.470	0.701	0.626	990	504	450	253	268			
56/44	0.267	0.450	0.657	0.619	840	477	423	246	258			
58/42	0.254	0.428	0.646	0.607	751	437	397	243	246			
60/40	0.238	0.400	0.625	0.585	672	410	376	240	245			
	$s_{11}^E$	$s_{11}^D$	$s_{33}^E$	$s_{33}^D$	$s_{44}^E$	$s_{44}^D$	$s_{66}$	$s_{12}^E$	$s_{12}^D$	$s_{13}^E$	$s_{13}^D$	Density $\rho$
	$10^{-12} \text{ m}^2 \text{ N}^{-1}$										$10^3 \text{ kgm}^{-3}$	
48/52	10.8	10.5	10.9	8.83	28.3	23.6	28.3	-3.35	-3.66	-3.21	-2.40	7.59
50/50	12.4	11.7	13.3	9.35	32.8	24.5	32.9	-4.06	-4.72	-4.22	-2.60	7.55
52/48	13.8	12.4	17.1	9.35	48.2	25.0	38.4	-4.07	-5.38	-5.80	-2.56	7.55
54/46	11.6	10.7	14.8	9.0	45.0	22.9	29.9	-3.33	-4.24	-4.97	-2.68	7.62
56/44	11.0	10.2	14.0	8.65	39.8	22.6	28.4	-3.22	-4.01	-4.63	-2.57	7.59
58/42	10.5	9.85	12.8	8.10	37.7	21.9	27.1	-3.07	-3.75	-4.12	-2.33	7.64
60/40	10.4	9.75	12.05	7.92	36.9	22.5	26.7	-2.96	-3.55	-3.72	-2.17	7.60
	$g_{31}$	$g_{33}$	$g_{15}$	$g_{33} - g_{31}$	$d_{31}$	$d_{33}$	$d_{15}$	$d_{33} - d_{31}$	$s_{33}^D + s_{11}^D$ $-2s_{13}^D$			
	$10^{-3} \text{ m}^2 \text{ C}^{-1}$				$10^{-12} \text{ C N}^{-1}$				$10^{-12} \text{ m}^2 \text{ N}^{-1}$			
48/52	-7.3	18.7	28.4	26.0	43.0	110	166	153	24.1			
50/50	-9.35	23.1	33.2	32.4	70.0	173	251	243	26.2			
52/48	-14.5	34.5	47.2	49.0	93.5	223	494	316	26.9			
54/46	-15.1	38.1	50.3	53.2	60.2	152	440	212	25.1			
56/44	-14.5	37.8	48.0	52.3	54.3	142	357	196	24.0			
58/42	-13.9	36.7	48.8	50.6	48.9	129	325	178	22.6			
60/40	-13.3	35.2	49.3	48.5	44.2	117	293	161	22.0			
	$Q_{\text{mech}}$	$Q_E$ (=1/ $\tan \delta$ )	$P$	$c_{33}^D$	$-s_{12}^E$	$-s_{12}^D$	$-s_{13}^E$	$-s_{13}^D$				
			$10^{-2} \text{ C m}^{-2}$	$10^{10} \text{ N m}^{-2}$	$s_{11}^E$	$s_{11}^D$	$\sqrt{s_{33}^E s_{11}^E}$	$\sqrt{s_{33}^D s_{11}^D}$				
48/52	1170	380	17	14.0	0.310	0.349	0.296	0.250				
50/50	950	370	27	13.5	0.328	0.404	0.329	0.249				
52/48	860	360	36	13.4	0.295	0.434	0.376	0.238				
54/46	680	300	42.5	14.8	0.288	0.396	0.380	0.273				
56/44	490	190	48	15.3	0.293	0.394	0.373	0.274				
58/42	500	200	43	15.8	0.292	0.381	0.355	0.261				
60/40	600	210	33	15.6	0.285	0.365	0.332	0.247				

Tab. 68.  $(\text{Pb}_{1-x}\text{Sr}_x)(\text{Zr}_{1-y}\text{Ti}_y)\text{O}_3$  and  $(\text{Pb}_{1-x}\text{Ca}_x)(\text{Zr}_{1-y}\text{Ti}_y)\text{O}_3$  (modified ceramics). Effects of Ca and Sr on electromechanical properties. [59K4]

Intended composition	$\rho_a$ $10^3$ kg m $^{-3}$	$x$ at 1 kHz	24 hours after poling						$\Theta_f$ °C
			$x$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$d_{31}$ $10^{-12}$ CN $^{-1}$	$\varepsilon_{31}$ $10^{-3}$ m $^2$ C $^{-1}$	$(s_{11}^E)^{-1}$ $10^{10}$ Nm $^{-2}$	
Pb( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.40	736	544	0.5	0.48	71	14.7	7.67	385
Pb( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.39	707	542	0.4	0.47	69	14.4	7.76	
Pb $_{0.59}\text{Ca}_{0.01}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.42	729	624	0.5	0.49	77	13.9	7.89	
Pb $_{0.59}\text{Sr}_{0.01}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.42	755	584	0.6	0.49	75	14.5	7.68	
Pb $_{0.55}\text{Ca}_{0.05}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.26	832	973	0.5	0.44	88	10.2	7.62	
Pb $_{0.55}\text{Sr}_{0.05}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.47	920	1002	0.4	0.50	101	11.4	7.65	360
Pb $_{0.52}\text{Ca}_{0.08}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	6.86	794	888	0.4	0.32	60	7.6	7.85	
Pb $_{0.52}\text{Sr}_{0.076}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.29	942	1094	0.3	0.50	103	10.6	7.94	
Pb $_{0.50}\text{Sr}_{0.10}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.22	997	1129	0.3	0.49	103	10.3	7.95	290
Pb $_{0.575}\text{Sr}_{0.125}$ ( $\text{Zr}_{0.47}\text{Ti}_{0.53}$ ) $\text{O}_3$	7.09	609	663	0.3	0.28	40	6.8	9.91	
Pb $_{0.875}\text{Sr}_{0.125}$ ( $\text{Zr}_{0.50}\text{Ti}_{0.50}$ ) $\text{O}_3$	7.11	813	880	0.3	0.33	57	7.3	9.05	
Pb $_{0.875}\text{Sr}_{0.125}$ ( $\text{Zr}_{0.52}\text{Ti}_{0.48}$ ) $\text{O}_3$	7.10	973	1149	0.3	0.44	91	9.0	8.32	
Pb $_{0.875}\text{Sr}_{0.125}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	7.14	1076	1237	0.4	0.47	100	9.1	8.06	265
Pb $_{0.875}\text{Sr}_{0.125}$ ( $\text{Zr}_{0.54}\text{Ti}_{0.46}$ ) $\text{O}_3$	7.16	1095	1325	0.6	0.51	119	10.1	7.51	
Pb $_{0.875}\text{Sr}_{0.125}$ ( $\text{Zr}_{0.56}\text{Ti}_{0.44}$ ) $\text{O}_3$	7.14	1105	1210	0.4	0.51	116	10.8	7.31	
Pb $_{0.875}\text{Sr}_{0.125}$ ( $\text{Zr}_{0.59}\text{Ti}_{0.41}$ ) $\text{O}_3$	7.17	919	585	0.4	0.45	66	12.7	8.39	
Pb $_{0.85}\text{Sr}_{0.15}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	6.90	1106	1260	0.5	0.43	97	8.7	7.68	242
Pb $_{0.80}\text{Sr}_{0.20}$ ( $\text{Zr}_{0.50}\text{Ti}_{0.50}$ ) $\text{O}_3$	6.56	941	970	0.6	0.29	56	6.5	8.11	
Pb $_{0.80}\text{Sr}_{0.20}$ ( $\text{Zr}_{0.53}\text{Ti}_{0.47}$ ) $\text{O}_3$	6.48	1212	1257	0.5	0.34	86	7.8	7.05	
Pb $_{0.80}\text{Sr}_{0.20}$ ( $\text{Zr}_{0.54}\text{Ti}_{0.46}$ ) $\text{O}_3$	6.36	1182	1341	0.8	0.35	91	7.7	6.18	
Pb $_{0.80}\text{Sr}_{0.20}$ ( $\text{Zr}_{0.55}\text{Ti}_{0.45}$ ) $\text{O}_3$	6.36	1200	1337	0.8	0.34	86	7.3	6.42	
Pb $_{0.80}\text{Sr}_{0.20}$ ( $\text{Zr}_{0.56}\text{Ti}_{0.44}$ ) $\text{O}_3$	6.35	1107	1113	0.7	0.35	81	8.2	6.50	

Tab. 69. Pb( $\text{Zr}-\text{Ti}$ ) $\text{O}_3$  (ceramics, modified). Electromechanical properties of Pb( $\text{Zr}_{0.54}\text{Ti}_{0.46}$ ) $\text{O}_3$  with five-valent additives. [59K5].  $f_R \cdot r$ : radial frequency constant

Addition wt. %	$\rho_a$ $10^3$ kg m $^{-3}$	Before poling		24 hours after poling						$\Theta_f$ °C
		$x$ at 1 kHz	$\tan \delta$ % at 1 kHz	$x$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$f_R \cdot r$ Hz $\cdot$ m	$d_{31}$ $10^{-12}$ CN $^{-1}$	$Q_{\text{mech}}$	
None	7.41	707	0.3	537	0.4	0.49	1641	71		390
None	7.29	706	0.4	513	0.5	0.50	1687	69		387
0.1 Nb $_2\text{O}_5$	7.26	598	0.3	508	0.4	0.38	1643	54		
0.5 Nb $_2\text{O}_5$	6.96	732	2.1	790	2.0	0.46	1443	94		
0.8 Nb $_2\text{O}_5$	7.36	965	1.6	1166	1.5	0.48	1606	105		
1.0 Nb $_2\text{O}_5$	7.36	1064	1.8	1308	1.6	0.53	1563	126	61	361
1.0 Nb $_2\text{O}_5$	7.60	1055	2.2	1242	2.2	0.54	1538	125		
1.2 Nb $_2\text{O}_5$	7.34	1011	2.0	1167	1.7	0.48	1614	104	70	
1.4 Nb $_2\text{O}_5$	7.37	1057	2.2	1218	1.9	0.50	1584	113	69	
1.7 Nb $_2\text{O}_5$	7.39	1058	2.0	1218	1.8	0.47	1594	105		
2.0 Nb $_2\text{O}_5$	7.37	1074	2.1	1202	2.0	0.50	1550	115		344
0.5 Nb $_2\text{O}_5$	7.39	1169	2.1	1377	2.0	0.57	1491	146	48	369
0.5 La $_2\text{O}_3$										
1.0 Ta $_2\text{O}_5$	7.31	989	1.5	1187	1.5	0.49	1563	111	61	
1.0 Ta $_2\text{O}_5$	7.22	918	2.0	1121	2.1	0.50	1525	114		368
2.0 Ta $_2\text{O}_5$	7.49	1062	2.2	1230	2.1	0.50	1547	115		
2.0 Ta $_2\text{O}_5$	7.40	1077	1.8	1275	1.8	0.48	1581	111		364
2.5 Ta $_2\text{O}_5$	7.23	959	2.7	1112	2.4	0.36	1518	82	28	
5.0 Ta $_2\text{O}_5$	6.75	995	2.5	1052	2.6	0.33	1508	76		

Tab. 70.  $\text{Pb}(\text{Zr}-\text{Ti})\text{O}_3$  (ceramics, modified). Electromechanical properties of  $\text{Pb}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$  with three-valent additives. [59K5].  $f_R \cdot r$ : radial frequency constant

Addition wt. %	$\rho_a$ $10^3$ $\text{kg m}^{-3}$	Before poling		24 hours after poling					$\Theta_f$ °C
		$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$f_R \cdot r$ Hz · m	$d_{31}$ $10^{-12}$ $\text{CN}^{-1}$	
None	7.41	707	0.3	537	0.4	0.49	1641	71	390
None	7.29	706	0.4	513	0.5	0.50	1687	69	387
1.0 $\text{Y}_2\text{O}_3$	7.26	796	0.9	841	1.0	0.34	1547	66	374
1.0 $\text{La}_2\text{O}_3$	7.46	1187	1.9	1483	2.0	0.53	1510	138	
1.0 $\text{La}_2\text{O}_3$	7.47	1139	2.2	1387	2.1	0.52	1522	130	339
1.0 $\text{Nd}_2\text{O}_3$	7.43	1111	1.6	1395	1.8	0.49	1512	123	
1.0 $\text{Nd}_2\text{O}_3$	7.37	1101	1.9	1354	1.8	0.48	1511	119	348
1.0 didymia	7.41	1122	2.2	1341	2.2	0.50	1499	125	
2.0 $\text{La}_2\text{O}_3$	7.49	1296	2.6	1545	2.3	0.51	1545	132	
1.0 $\text{La}_2\text{O}_3$	7.20	1375	2.1	1792	1.7	0.51	1528	147	
1.0 $\text{Nd}_2\text{O}_3$	7.35	1362	2.2	1776	1.9	0.49	1558	136	
0.1 $\text{La}_2\text{O}_3$	6.75	790	0.4	870	0.6	0.42	1505	88	
0.2 $\text{La}_2\text{O}_3$	6.45	686	0.7	735	0.9	0.37	1419	78	
0.4 $\text{La}_2\text{O}_3$	6.44	942	1.4	1100	1.5	0.42	1407	109	
0.8 $\text{La}_2\text{O}_3$	7.19	1288	1.8	1682	1.8	0.49	1516	139	
1.0 $\text{La}_2\text{O}_3$	7.50	1255	2.4	1532	2.4	0.50	1550	128	

Tab. 71. Electromechanical properties of  $\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$  (ceramics), modified with additives of 1 wt% Nb. [59K5].  $f_R \cdot r$ : radial frequency constant

Base composition	$\rho_a$ $10^3$ $\text{kg m}^{-3}$	Before poling		24 hours after poling					$Q_{\text{mech}}$
		$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$f_R \cdot r$ Hz · m	$d_{31}$ $10^{-12}$ $\text{CN}^{-1}$	
$\text{Pb}(\text{Zr}_{0.50}\text{Ti}_{0.50})\text{O}_3$	7.38	879	1.5	1041	1.2	0.42	1696	82	81
$\text{Pb}(\text{Zr}_{0.51}\text{Ti}_{0.49})\text{O}_3$	7.31	975	1.6	1188	1.3	0.45	1642	97	73
$\text{Pb}(\text{Zr}_{0.52}\text{Ti}_{0.48})\text{O}_3$	7.39	985	1.5	1200	1.4	0.45	1640	97	76
$\text{Pb}(\text{Zr}_{0.53}\text{Ti}_{0.47})\text{O}_3$	7.43	1092	1.8	1371	1.4	0.53	1547	130	61
$\text{Pb}(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$	7.44	1051	1.8	1296	1.7	0.54	1549	128	62
$\text{Pb}(\text{Zr}_{0.55}\text{Ti}_{0.45})\text{O}_3$	7.40	955	2.4	973	2.0	0.56	1524	117	55
$\text{Pb}(\text{Zr}_{0.56}\text{Ti}_{0.44})\text{O}_3$	7.38	818	2.8	745	2.5	0.53	1601	93	56
$\text{Pb}(\text{Zr}_{0.57}\text{Ti}_{0.43})\text{O}_3$	7.41	750	3.0	684	2.5	0.50	1636	82	60
$\text{Pb}(\text{Zr}_{0.58}\text{Ti}_{0.42})\text{O}_3$	7.41	713	3.0	630	2.8	0.49	1676	75	62

Tab. 72. Electromechanical properties of  $(\text{Pb}_{0.95}\text{Sr}_{0.05})(\text{Zr}_{0.54}\text{Ti}_{0.46})\text{O}_3$  (ceramics) with  $\text{Nb}_2\text{O}_5$  or  $\text{Ta}_2\text{O}_5$ . [59K5].  $f_R \cdot r$ : radial frequency constant

Addition wt. %	$\rho_a$ $10^3$ $\text{kg m}^{-3}$	Before poling		24 hours after poling					$\Theta_f$ °C
		$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$\kappa$ at 1 kHz	$\tan \delta$ % at 1 kHz	$k_p$	$f_R \cdot r$ Hz · m	$d_{31}$ $10^{-12}$ $\text{CN}^{-1}$	
1.0 $\text{Nb}_2\text{O}_5$	7.34	1291	2.0	1609	2.0	0.56	1512	153	306
2.0 $\text{Nb}_2\text{O}_5$	7.22	1380	2.4	1662	2.1	0.47	1562	127	
3.0 $\text{Nb}_2\text{O}_5$	6.63	1125	2.1	1301	2.1	0.36	1550	91	
2.0 $\text{Ta}_2\text{O}_5$	7.33	1343	2.3	1695	2.0	0.54	1517	151	296

-ith	
$\theta_f$	
°C	
90	
87	
74	
339	
348	
% Nb.	
$Q_{\text{mech}}$	
81	
73	
76	
61	
62	
55	
56	
60	
62	
r Ta <sub>2</sub> O <sub>5</sub>	
$\theta_f$	
°C	
306	
296	

Tab. 73. PZT (commercial modified ceramics). Electromechanical constants at RT. [66b1]

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Nr. 1C-a29 $\text{PbTiO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 555, 556
Nr. 1C-a30 $\text{PbTiO}_3\text{-PbO:SnO}_2$	1b   Phase diagram: Fig. 557. 5a   Dielectric constant: Fig. 558.
Nr. 1C-a31 $\text{PbZrO}_3\text{-PbHfO}_3$	1b   Phase diagram: Fig. 559.
Nr. 1C-a32 $\text{PbZrO}_3\text{-PbO:SnO}_2$	1b   Phase diagram: Fig. 560. Lattice parameter: Fig. 561. 4   Thermal expansion: Fig. 562, 563. 5a   Dielectric constant: Fig. 564a, b.
Nr. 1C-a33 $\text{LaFeO}_3\text{-BiFeO}_3$	1b   Phase diagram: Fig. 565. Lattice parameter: Fig. 566a, b. 5a   Dielectric constant: Fig. 567. 11   Magnetization: see Fig. 565.
Nr. 1C-b1 $\text{NaNbO}_3\text{-KTaO}_3$	1b   Phase diagram: Fig. 568. Lattice parameter: Fig. 569. 4   Thermal expansion: Fig. 570. 5a   Dielectric constant: Fig. 571.
Nr. 1C-b2 $\text{NaNbO}_3\text{-KSbO}_3$	1a   Curie temperature: see Fig. 423.
Nr. 1C-b3 $\text{BaTiO}_3\text{-PbZrO}_3$	4   Thermal expansion: Fig. 572. 5a   Dielectric constant: Fig. 573.
Nr. 1C-b4 $\text{BaTiO}_3\text{-PbO:SnO}_2$	1b   Phase diagram: Fig. 574. 5a   Dielectric constant: Fig. 575.
Nr. 1C-b5 $\text{PbTiO}_3\text{-CaZrO}_3$	1b   Phase diagram: Fig. 576. Lattice parameter: Fig. 577. 5a   Dielectric constant: Fig. 578.
Nr. 1C-b6 $\text{PbTiO}_3\text{-CaSnO}_3$	1b   Phase diagram: see Fig. 576. Lattice parameter: Fig. 579. 5a   Dielectric constant: Fig. 580.
Nr. 1C-b7 $\text{PbTiO}_3\text{-SrZrO}_3$	1b   Phase diagram: Fig. 581. Lattice parameter: Fig. 582a, b. 5a   Dielectric constant: Fig. 583.
Nr. 1C-b8 $\text{PbTiO}_3\text{-SrSnO}_3$	1b   Phase diagram: Fig. 584. Lattice parameter: Fig. 585a, b. 5a   Dielectric constant: Fig. 586.
Nr. 1C-b9 $\text{PbTiO}_3\text{-BaZrO}_3$	1b   Phase diagram: Fig. 587. Lattice parameter: Fig. 588a, b. 5a   Dielectric constant: Fig. 589. 7a   Electromechanical property: Tab. 74.

Tab. 74.  $(1 - x)\text{PbTiO}_3 - x\text{BaZrO}_3$  (ceramics).  $k_p$  and  $d_{33}$  at RT. [63B15]

$x$	Poling field $\cdot 10^5 \text{ V m}^{-1}$ [ $T$ in $^\circ\text{C}$ ]	$k_p$	$d_{33}$ $\cdot 10^{-12} \text{ C N}^{-1}$
0.25	29 [185 ... 40]	0.16	40
0.30	27 [170 ... 40]	0.23	50
0.35	39 [145 ... 40]	0.30	110
0.40	30 [120 ... 40]	0.17	45

Nr. 1C-b10 $\text{PbTiO}_3\text{-BaSnO}_3$	1b   Phase diagram: Fig. 590. Lattice parameter: Fig. 591a, b.
Nr. 1C-b11 $\text{LaAlO}_3\text{-BiFeO}_3$	1b   Phase diagram: Fig. 592. Lattice parameter: Fig. 593.
	5a   Dielectric constant: Fig. 594.
Nr. 1C-b12 $\text{LaCrO}_3\text{-BiFeO}_3$	1b   Phase diagram: Fig. 595. Lattice parameter: Fig. 596a, b.
	4   Thermal expansion: Fig. 597.
	11   Spontaneous magnetization: see Fig. 595.
Nr. 1C-c1 $\text{NaNbO}_3\text{-CaTiO}_3$	1b   Phase diagram: Fig. 598.
	5a   Dielectric constant: Fig. 599.
Nr. 1C-c2 $\text{NaNbO}_3\text{-BaTiO}_3$	1b   Phase diagram: Fig. 600.
Nr. 1C-c3 $\text{NaNbO}_3\text{-PbTiO}_3$	1b   Transition temperature: Fig. 601.
	5a   Dielectric constant: Fig. 602.
Nr. 1C-c4 $\text{NaNbO}_3\text{-PbZrO}_3$	1b   Phase diagram: Fig. 603.
	5a   Dielectric constant: Fig. 604a, b.
Nr. 1C-c5 $\text{KNbO}_3\text{-BaTiO}_3$	1b   Phase diagram: Fig. 605. Lattice parameter: Fig. 606.
	5a   Dielectric constant: Fig. 607a, b, c.
Nr. 1C-c6 $\text{KNbO}_3\text{-PbTiO}_3$	1b   Phase diagram: Fig. 608. Lattice parameter: Fig. 609.
	5a   Dielectric constant: Fig. 610a, b.
Nr. 1C-c7 $\text{SrTiO}_3\text{-BiFeO}_3$	1b   Phase diagram: Fig. 611. Lattice parameter: Fig. 612.
	5a   Relaxation phenomena are observed in the range II [65F1].
Nr. 1C-c8 $\text{BaTiO}_3\text{-LaAlO}_3$	1b   Lattice parameter and Curie temperature: Tab. 75.

Tab. 75.  $\text{BaTiO}_3\text{-LaAlO}_3$ . Lattice parameters and  $\Theta_f$ . [58I4]

Concentration mol%		$a$ Å	$c$ Å	$c/a$	$V$ Å <sup>3</sup>	$\Theta_f$ °C
$\text{BaTiO}_3$	$\text{LaAlO}_3$					
100.0	—	3.9956	4.0352	1.0100	64.42	+120
99.0	1.0	3.9951	4.0345	1.0098	64.39	+ 87
97.5	2.5	3.9949	4.0293	1.0086	64.30	+ 46
95.0	5.0	4.0050	—	1.0000	64.24	- 14
92.5	7.5	4.0011	—	1.0000	64.05	- 85
90.0	10.0	3.9984	—	1.0000	63.92	-133
87.5	12.5	3.9950	—	1.0000	63.76	—
85.0	15.0	3.9906	—	1.0000	63.55	—
75.0	25.0	3.9800	—	1.0000	63.04	—
—	100.0	3.7950	—	1.000	54.65	—

Nr. 1C-c9  $\text{BaTiO}_3\text{-BiFeO}_3$ 11 | Néel temperature and magnetic resonance line width:  
12 | Fig. 613.Nr. 1C-c10  $\text{PbTiO}_3\text{-LaAlO}_3$ 1b | Phase diagram: Fig. 614.  
Lattice parameter: Fig. 615.  
5a | Dielectric constant: Fig. 616.Nr. 1C-c11  $\text{PbTiO}_3\text{-LaMnO}_3$ 1b | Transition temperatures: Fig. 617.  
Lattice parameters: Fig. 618.Nr. 1C-c12  $\text{PbTiO}_3\text{-LaFeO}_3$ 1b | Phase diagram: Fig. 619.  
Lattice parameter: Fig. 620.  
5a | Dielectric constant: Fig. 621.Nr. 1C-c13  $\text{PbTiO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 622a, b.  
Lattice parameter: Fig. 623a, b.  
4 | Thermal expansion: Fig. 624.  
5a | Dielectric constant: Fig. 625.Nr. 1C-c14  $\text{PbZrO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 626.  
Lattice parameter: Fig. 627.  
5a | Dielectric constant: Fig. 628.Nr. 1C-c15  $\text{SrSnO}_3\text{-BiFeO}_3$ 1b | Phase diagram: Fig. 629.  
12c | Mössbauer absorption: Fig. 630.Nr. 1C-c16  $\text{SrFeO}_3\text{-BiFeO}_3$ 1a | Unit cell volume: Fig. 631.  
11 | Magnetization: Fig. 632.Nr. 1C-d1  $\text{SrTiO}_3\text{-Sr}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$ 

1b | Phase diagram: Fig. 633.

Nr. 1C-d2  $\text{BaTiO}_3\text{-Ba}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$ 

2b | Phase diagram: Fig. 634.

Nr. 1C-d3  $\text{BaTiO}_3\text{-}(\text{K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$ 1b | Curie temperature: Fig. 635.  
Lattice parameters: Fig. 636.Nr. 1C-d4  $\text{PbTiO}_3\text{-}(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$ 1b | Phase diagram and lattice parameters: Fig. 637.  
5a | Dielectric constant: Fig. 638.Nr. 1C-d5  $\text{PbTiO}_3\text{-}(\text{K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$ 

1b | Curie temperature and lattice parameters: Fig. 639.

Nr. 1C-d6  $\text{PbTiO}_3\text{-}(\text{Li}_{1/2}\text{La}_{1/2})\text{TiO}_3$ 

1b | Curie temperature and lattice parameters: Fig. 640.

Nr. 1C-d7 $\text{PbTiO}_3\text{-}(\text{Na}_{1/2}\text{La}_{1/2})\text{TiO}_3$	1b   Curie temperature and lattice parameters: Fig. 641.
Nr. 1C-d8 $\text{PbTiO}_3\text{-}(\text{Li}_{1/2}\text{Ce}_{1/2})\text{TiO}_3$	1b   Lattice parameters: Fig. 642.
Nr. 1C-d9 $\text{PbTiO}_3\text{-}(\text{Li}_{1/2}\text{Nd}_{1/2})\text{TiO}_3$	1b   Lattice parameters: Fig. 643.
Nr. 1C-d10 $\text{PbTiO}_3\text{-Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3$	1b   Phase diagram: Fig. 644. Lattice parameters: Fig. 645.
Nr. 1C-d11 $\text{PbTiO}_3\text{-Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$	1b   Curie temperature: Fig. 646.
Nr. 1C-d12 $\text{PbTiO}_3\text{-Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Curie temperature: Fig. 647.
Nr. 1C-d13 $\text{PbTiO}_3\text{-Pb}(\text{Mn}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Transition temperature: Fig. 648. Lattice parameters: Fig. 649.
Nr. 1C-d14 $\text{PbZrO}_3\text{-Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Curie temperature: see Fig. 647.
Nr. 1C-d15 $\text{PbZrO}_3\text{-Pb}(\text{Fe}_{1/2}\text{Ta}_{1/2})\text{O}_3$	1b   Curie temperature: Fig. 650.
Nr. 1C-d16 $\text{PbZrO}_3\text{-}(\text{Na}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$	1b   Phase diagram: Fig. 651. 4   Lattice distortion: Fig. 652. 5a   Dielectric constant: Fig. 653.
Nr. 1C-d17 $\text{PbZrO}_3\text{-}(\text{K}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$	1b   Phase diagram: Fig. 654. Lattice parameters: Tab. 76. 4   Lattice distortion: Fig. 655. 5a   Dielectric constants: Fig. 656.

Tab. 76.  $(1 - x)\text{PbZrO}_3 - x(\text{K}_{1/2}\text{Bi}_{1/2})\text{ZrO}_3$ . Lattice constants at RT [62B10]

$x$	$a$ Å	$b$ Å	$c$ Å	
0	5.884	11.768	8.220	orthorhombic
0.10	5.882	11.764	8.227	orthorhombic
0.20	5.877	11.755	8.237	orthorhombic
0.30	5.876	11.751	8.248	orthorhombic
0.40	4.151	—	—	cubic
0.50	4.152	—	—	cubic

Nr. 1C-d18 $\text{PbHfO}_3\text{-Pb}(\text{Sc}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Curie temperature: see Fig. 647.
Nr. 1C-d19 $\text{Pb}(\text{Mg}_{1/2}\text{W}_{1/2})\text{O}_3\text{-Pb}(\text{Mg}_{1/3}\text{Nb}_{2/3})\text{O}_3$	1b   Phase diagram: Fig. 657.
Nr. 1C-d20 $(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3\text{-}(\text{K}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1b   Curie temperature: see Fig. 635. Lattice parameters: see Fig. 636.
Nr. 1C-d21 $\text{PbZrO}_3\text{-}(\text{Na}_{1/2}\text{Bi}_{1/2})\text{TiO}_3$	1b   Phase diagram: Fig. 658. Lattice parameters: Fig. 659.
Nr. 1C-d22 $\text{BiFeO}_3\text{-Sr}(\text{Sn}_{1/3}\text{Mn}_{2/3})\text{O}_3$	1b   Phase diagram: Fig. 660. Lattice parameters: Fig. 661. 12c   Mössbauer effect: see [65M8]
Nr. 1C-d23 $\text{BiFeO}_3\text{-Pb}(\text{Fe}_{1/2}\text{Nb}_{1/2})\text{O}_3$	1b   Lattice parameters: Fig. 662. 5a   Dielectric constant: Fig. 663. 11   Magnetic susceptibility: Fig. 664. Néel temperature and spontaneous magnetization: Fig. 665.

**Nr. 1C-e1  $\text{NaNbO}_3\text{-LiNbO}_3$** 

1b	Phase diagram: Fig. 666.
5a	Dielectric constant: Fig. 667.

**Nr. 1C-e2  $\text{NaNbO}_3\text{-NaVO}_3$** 

5a	Dielectric constant: Fig. 668.
14b	Switching: see Fig. 9.

**Nr. 1C-e3  $\text{NaNbO}_3\text{-CaNb}_2\text{O}_6$** 

1b	Phase diagram: Fig. 669.
5a	Dielectric constant: Fig. 670.

**Nr. 1C-e4  $\text{NaNbO}_3\text{-CdNb}_2\text{O}_6$** 

1b	Phase diagram: Fig. 671, 672. Lattice parameter: Fig. 673.
5a	Dielectric constant: Fig. 674; Tab. 77.
7a	Piezoelectricity: Fig. 675; Tab. 78.

Tab. 77.  $(1 - x)\text{NaNbO}_3 - (x/2)\text{CdNb}_2\text{O}_6$  [56L2].  $r$ : capacitance ratio;  $C$ : Curie constant;  $\Theta_f$ ,  $\Theta$  compare Fig. 671, 672

Composition $x$	Firing conditions			$x_{RT}$	$r$	$\Theta$ °C	$x_{\max}$	$\Theta_f$ °C	$C \cdot 10^4$ °C	$\Theta_p$ °C	$\rho$ $10^8 \text{ kg m}^{-3}$
	T °C	t hr	atmosphere								
0.02	1250	1	CdO	230	—	200	2700	375	12	345	3.9
0.05	1250	1	CdO	500	1200	60	4000	375	12	345	4.2
0.10	1250	1	CdO	1000	130	75	4100	320	18	275	4.3
0.15	1250	1	CdO	1400	40	50	8500	285	24	260	4.3
0.20	1250	1	CdO	2300	20	20	10000	250	14	250	4.4
0.25	1250	1	CdO	3500	10	5	15000	220	20	230	4.5
0.30	1220	2	CdO	2700	12	—25	11000	210	20	205	4.6

Tab. 78.  $(1 - x)\text{NaNbO}_3 - (x/2)\text{CdNb}_2\text{O}_6$  (ceramics) [62K4]

$x$	0.05	0.10	0.15	0.20	0.25	0.30	
$\rho$	4.2	4.3	4.3	4.3	4.4	4.2	$10^8 \text{ kg m}^{-3}$
$f_R \cdot 2r$	3.0	3.0	3.0	3.15	3.36	3.25	$10^3 \text{ Hz m}$
$s_{11}^E$	11.9	11.6	11.6	10.5	9.0	10.1	$10^{-12} \text{ m}^2 \text{ N}^{-1}$
$\tan \delta$	0.01	0.01	0.02	0.01	0.01	0.03	
$x$ at $\Theta_f$	4	4.1	8.5	16	13	11	$10^8$

**Nr. 1C-e5  $\text{NaNbO}_3\text{-SrNb}_2\text{O}_6$** 

1b	Phase diagram: Fig. 676. Lattice parameter: Fig. 677.
5a	Dielectric constant: Fig. 678.
7a	Electromechanical properties: Fig. 679, 680, 681.

**Nr. 1C-e6  $\text{NaNbO}_3\text{-PbNb}_2\text{O}_6$** 

1b	Phase diagram: Fig. 682. Lattice parameter: Fig. 683.
7a	Electromechanical properties: Fig. 684.

**Nr. 1C-e7  $\text{CdTiO}_3\text{-LiNbO}_3$ ,  $\text{CdTiO}_3\text{-LiTaO}_3$** 

5a	Dielectric constant: Fig. 685.
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**Nr. 1C-e8  $\text{SrTiO}_3\text{-Bi}_2\text{O}_3 \cdot 3\text{TiO}_2$** 

1b	Lattice parameter: Fig. 686.
5a	Dielectric constant: Fig. 687, 688.

**Nr. 1C-e9  $\text{BaTiO}_3\text{-BaNb}_2\text{O}_6$** 

1b	Phase diagram: Fig. 689.
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Nr. 1C-e10 BaTiO <sub>3</sub> -BaTa <sub>2</sub> O <sub>6</sub>	1b   Lattice parameter: Fig. 690. 5a   Dielectric constant: Fig. 691.
Nr. 1C-e11 BaTiO <sub>3</sub> -A <sub>2</sub> B <sub>2</sub> O <sub>7</sub>	1b   Curie temperature: Fig. 692. 5a   Dielectric constant: Fig. 693 ... 697.
Nr. 1C-e12 PbZrO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	
For the solid solution with PbNb <sub>2</sub> O <sub>6</sub> as an end material see 5B-8.	
	1b   Phase diagram: Fig. 698. 4   Thermal expansion: Fig. 699. 5   Dielectric constant: Fig. 700.
Nr. 1C-e13 PbZrO <sub>3</sub> -PbTa <sub>2</sub> O <sub>6</sub>	1b   Phase diagram: Fig. 701. 4   Thermal expansion: see Fig. 699. 5   Dielectric constant: Fig. 702.
Nr. 1C-f1 CaTiO <sub>3</sub> -SrTiO <sub>3</sub> -BaTiO <sub>3</sub>	1b   Phase diagram: Fig. 703.
Nr. 1C-f2 CaTiO <sub>3</sub> -BaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1b   Phase diagram: Fig. 704, 705. Curie temperature: Fig. 706. 7a   Electromechanical properties: see Nr. 1A-8, 7a.
Nr. 1C-f3 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -PbO:SnO <sub>2</sub>	1b   Phase diagram: Fig. 707. 8b   Elastic properties: Fig. 708, 709.
Nr. 1C-f4 PbTiO <sub>3</sub> -PbHfO <sub>3</sub> -PbO:SnO <sub>2</sub>	1b   Phase diagram: Fig. 710.
Nr. 1C-f5 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -LaFeO <sub>3</sub>	1b   Phase diagram: Fig. 711. Lattice parameters: Fig. 712.
Nr. 1C-f6 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -BiFeO <sub>3</sub>	1b   Phase diagram: Fig. 713. Lattice parameters: Fig. 714.
Nr. 1C-f7 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1b   Phase diagram: Fig. 715. Lattice parameters: Fig. 716. 7a   Electromechanical property: Fig. 717, 718.
Nr. 1C-f8 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1b   Lattice parameters: Fig. 719. Curie temperature: Fig. 720. 7a   Electromechanical property: Fig. 721.
Nr. 1C-f9 PbTiO <sub>3</sub> -PbZrO <sub>3</sub> -ABO <sub>3</sub>	1b   Phase diagram: Fig. 722.
Nr. 1C-f10 PbTiO <sub>3</sub> -SrTiO <sub>3</sub> -LaMnO <sub>3</sub>	1b   Curie temperature: Fig. 723.
Nr. 1C-f11 PbTiO <sub>3</sub> -LaMnO <sub>3</sub> -LaMeO <sub>3</sub> , (Me = Fe, Co, Ni, Cr)	
	1b   Transition temperatures: Fig. 724. 5a   Dielectric constant: Fig. 725. 11   Magnetic susceptibility: see Fig. 725. Magnetization: Fig. 726.

Figuren S. 349 ff.

II 2 WO<sub>3</sub>

Nr. 1C-f12 BaTiO <sub>3</sub> -SrTiO <sub>3</sub> -LaYO <sub>3</sub> -LaInO <sub>3</sub>	1b   Phase diagram: Fig. 727.
Nr. 1C-f13 CaSnO <sub>3</sub> -SrSnO <sub>3</sub> -BaSnO <sub>3</sub>	1b   Phase diagram: Fig. 728.
Nr. 1C-f14 (Na-K)(Nb-Ta)O <sub>3</sub>	1b   Phase diagram: Fig. 729.
Nr. 1C-f15 (Ca-Ba)(Ti-Zr)O <sub>3</sub>	1b   Phase diagram: Fig. 730.
Nr. 1C-f16 (Sr-Pb)(Ti-Zr)O <sub>3</sub>	1b   Phase diagram: Fig. 731. Lattice parameter: Fig. 732. Transition temperature: Fig. 733. 5a   Dielectric constant: Fig. 734, 735.
Nr. 1C-f17 (Ba-Pb)(Ti-Zr)O <sub>3</sub>	1b   Phase diagram: Fig. 736. Lattice parameter: Fig. 737. Transition temperature: Fig. 738. 7a   Electromechanical properties: Fig. 739, 740.
Nr. 1C-f18 (Ba-Pb)(Ti-Sn)O <sub>3</sub>	1b   Phase diagram: Fig. 741, 742. Lattice parameter: Fig. 743. Transition temperature: Fig. 744.
Nr. 1C-f19 BaTiO <sub>3</sub> -PbTiO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1b   Phase diagram: Fig. 745. Lattice parameter: Fig. 746.

## 2 WO<sub>3</sub>

### 2A Pure compound

#### Nr. 2A-1 WO<sub>3</sub>, Tungsten trioxide

1a	The anomalous dielectric properties of ceramic specimens of WO <sub>3</sub> were discovered by OGAWA <sup>a)</sup> in 1948. Possibility of ferroelectricity in WO <sub>3</sub> was pointed out by MATTHIAS <sup>b)</sup> in 1949.								<sup>a)</sup> 48N1, 48N2 <sup>b)</sup> 49M2
b	phase	VII	VI	V	IV	III	II	I	<sup>a)</sup> 49M2
	state	F <sup>e)</sup>							<sup>b)</sup> 60T1
	crystal system	mono-clinic <sup>*b)</sup>	tri-clinic <sup>b)</sup>	mono-clinic <sup>c)</sup>	ortho-rhombic <sup>b)</sup>	tetragonal <sup>d)</sup>	tetragonal <sup>b)</sup>	tetragonal <sup>b)</sup>	<sup>c)</sup> 60T2
	space group			P2 <sub>1</sub> /n <sup>c)</sup> -C <sub>2h</sub> <sup>c)</sup>		P4/nmm <sup>d)</sup> -D <sub>4h</sub> <sup>d)</sup>			<sup>d)</sup> 52K1
	Θ	-40 <sup>b)</sup>	17 <sup>b)</sup>	330 <sup>e)</sup>	740 <sup>e)</sup>	910 <sup>e)</sup>	1230 <sup>e)</sup>	°C	<sup>e)</sup> 56S1
	<i>T<sub>melt</sub> = 1473 °C. ρ = 7.157 · 10<sup>3</sup> kg m<sup>-3</sup> at RT. a = 7.30 Å, b = 7.53 Å, c = 7.68 Å, β = 90° 54' at 30 °C. Transparent, bluish green.</i>								21J1 04S1 60T1
2a	Crystal growth: Sublimation method.								51U1, 56T2, 59S3
b	Crystal form: Plate-like.								51U1, 56T2, 59S3
3	Crystal structure: Fig. 747, 748; Tab. 79; Fig. 749.								60T1
	phase	VII	VI	V	IV	III	II	I	
	Z	4	8	8					
4	Lattice distortion: Tab. 80. Thermal expansion: Fig. 750 ... 754.								
5a	Dielectric constant: $\kappa = 100 \dots 300$ at liquid air temperature. No reliable dielectric measurements could be carried out at and above room temperature because of high electrical conductivity. $d\Theta_{IV-III}/dp = -8.46 \cdot 10^{-8} \text{ K N}^{-1} \text{ m}^2$ .								49M2
c	Dielectric hysteresis loop was observed at liquid air temperature.								66T4 49M2

\* As to the crystal system in the phase VII, possibility of triclinic symmetry was discussed by TANISAKI [60T1].

## V Index of substances — Substanzenverzeichnis

This index consists of two parts: part A is for pure compounds (including complex compounds such as  $\text{Pb}(\text{Co}_{1/2}\text{Nb}_{1/2})\text{O}_8$  or  $\text{Na}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$ ) and part B is for solid solutions.

V A: In the 1st column the substances are ordered according to the alphabetically arranged gross formula. When their names (e.g. Rochelle salt) and/or their abbreviated names (e.g. TGS) are widely used, they are also included in this column. In the gross formula the numbers of the elements are determined by simple addition.

Compounds containing water of crystallization are, however, listed twice: (1) H and O of the water molecules are included in the gross formula, (2) the water molecules are attached separately to the gross formula. For instance, Rochelle salt is listed in the 1st column as  $\text{C}_4\text{H}_4\text{KNaO}_6 \cdot 4\text{H}_2\text{O}$ ,  $\text{C}_4\text{H}_{12}\text{KNaO}_{10}$  and also as Rochelle salt, RS, Seignette salt.

Crystals in which H is replaced by D (e.g.  $\text{KD}_2\text{PO}_4$ ) are not listed separately, since data on their properties are presented in the same section as the data on the non-deuterated crystals (e.g.  $\text{KH}_2\text{PO}_4$ ).

V B: In the 1st column the gross formula of each end material of a solid solution (e.g.  $\text{BaTiO}_3$  or  $\text{PbTiO}_3$  for the solid solution  $\text{BaTiO}_3-\text{PbTiO}_3$ ) is listed in the same manner as in the case of pure compounds. Thus the solid solution  $\text{BaTiO}_3-\text{PbTiO}_3$  can be found in the 2nd column by looking first for either  $\text{BaO}_3\text{Ti}$  or  $\text{O}_3\text{PbTi}$  in the 1st column of Part B. If the solid solution is expressed by the formula such as  $(\text{Sb}_x\text{Bi}_{1-x})\text{SI}$ , the end material can be obtained by putting  $x$  equal to either 0 or 1. When solid solutions have abbreviated names (e.g. KTN), these are also included in the 1st column.

Since in general one section corresponds to one substance in this volume, the 3rd column gives the section number and the 4th column gives the first page of the section.

Dieses Verzeichnis besteht aus zwei Teilen: Teil A enthält die reinen Verbindungen (einschließlich komplexer Verbindungen wie  $\text{Pb}(\text{Co}_{1/2}\text{Nb}_{1/2})\text{O}_8$  oder  $\text{Na}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$ ) und Teil B enthält die Mischkristalle.

V A: In der 1. Spalte sind die Substanzen nach der alphabetisch angeordneten Bruttoformel aufgeführt. Wenn ihre Namen (z. B. Seignette-Salz) und/oder ihre abgekürzten Bezeichnungen (z. B. TGS) häufig gebraucht werden, sind auch sie in dieser Spalte zu finden. In der Bruttoformel ist die Anzahl jedes Elements durch einfache Addition bestimmt.

Verbindungen, die Kristallwasser enthalten, sind zweimal aufgeführt: 1. H und O der Wassermoleküle sind in der Bruttoformel enthalten. 2. die Wassermoleküle werden getrennt der Bruttoformel hinzugefügt (z. B. Seignette-Salz ist in der 1. Spalte aufgeführt als  $\text{C}_4\text{H}_4\text{KNaO}_6 \cdot 4\text{H}_2\text{O}$ ,  $\text{C}_4\text{H}_{12}\text{KNaO}_{10}$  und auch als Rochelle-Salz, RS, Seignette-Salz).

Kristalle, in denen H durch D ersetzt ist (z. B.  $\text{KD}_2\text{PO}_4$ ), werden nicht gesondert aufgeführt. Daten von ihren Eigenschaften erscheinen in demselben Abschnitt an der gleichen Stelle wie die Daten von den nicht deuterierten Kristallen (z.B.  $\text{KH}_2\text{PO}_4$ ).

V B: In der 1. Spalte ist die Bruttoformel jeder Endsubstanz einer Mischkristallreihe (z. B.  $\text{BaTiO}_3$  oder  $\text{PbTiO}_3$  für die Mischkristallreihe  $\text{BaTiO}_3-\text{PbTiO}_3$ ) in derselben Weise aufgeführt wie im Fall von reinen Verbindungen. So kann die Mischkristallreihe  $\text{BaTiO}_3-\text{PbTiO}_3$  in der zweiten Spalte gefunden werden, wenn man zunächst entweder  $\text{BaO}_3\text{Ti}$  oder  $\text{O}_3\text{PbTi}$  in der ersten Spalte von Teil B sucht. Wenn die Mischkristallreihe durch die Formel  $(\text{Sb}_x\text{Bi}_{1-x})\text{SI}$  ausgedrückt wird, kann man die Endsubstanz finden, indem man  $x$  gleich 0 oder 1 setzt. Wenn Mischkristalle abgekürzte Namen haben (z. B. KTN), sind diese auch in der 1. Spalte enthalten.

Da in diesem Band jeweils ein Abschnitt einer Substanz entspricht, gibt die 3. Spalte die Abschnittsnr. und die 4. Spalte die erste Seite des Abschnitts an.

## VA Pure compounds

Gross formula	Chemical formula	Nr.	Page
ADP	$\text{NH}_4\text{H}_2\text{PO}_4$	13A-7	143
$\text{AgC}_2\text{H}_5\text{N}_2\text{O}_5$	$\text{NH}_3\text{CH}_2\text{COOH} \cdot \text{AgNO}_3$	29A-1	191
$\text{Ag}_2\text{H}_3\text{IO}_6$	$\text{Ag}_2\text{H}_3\text{IO}_6$	35-22	209
$\text{AgNbO}_3$	$\text{AgNbO}_3$	35-16	207
$\text{AgO}_3\text{Ta}$	$\text{AgTaO}_3$	35-18	207
$\text{AgO}_3\text{V}$	$\text{AgVO}_3$	35-20	208
$\text{AlCH}_6\text{NO}_8\text{S}_2 \cdot 12\text{H}_2\text{O}$	$\text{CH}_3\text{NH}_3\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-4	158
$\text{AlCH}_6\text{N}_3\text{O}_8\text{S}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}(\text{NH}_3)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-1	161
$\text{AlCH}_{18}\text{N}_3\text{O}_{14}\text{S}_2$	$\text{C}(\text{NH}_3)_3\text{Al}(\text{SO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-1	161
$\text{AlCH}_{30}\text{NO}_{20}\text{S}_2$	$\text{CH}_3\text{NH}_3\text{Al}(\text{SO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-4	158
$\text{AlCH}_6\text{NO}_8\text{Se}_2 \cdot 12\text{H}_2\text{O}$	$\text{CH}_3\text{NH}_3\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-10	161
$\text{AlCH}_6\text{N}_3\text{O}_8\text{Se}_2 \cdot 6\text{H}_2\text{O}$	$\text{C}(\text{NH}_3)_3\text{Al}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-5	166
$\text{AlCH}_{18}\text{N}_3\text{O}_{14}\text{Se}_2$	$\text{C}(\text{NH}_3)_3\text{Al}(\text{SeO}_4)_2 \cdot 6\text{H}_2\text{O}$	19A-5	166
$\text{AlCH}_{30}\text{NO}_{20}\text{Se}_2$	$\text{CH}_3\text{NH}_3\text{Al}(\text{SeO}_4)_2 \cdot 12\text{H}_2\text{O}$	18A-10	161
Ammonium metaphosphate			
$\text{AsCsH}_2\text{O}_4$	$\text{CsH}_2\text{AsO}_4$	35-14	205
$\text{AsH}_2\text{KO}_4$	$\text{KH}_2\text{AsO}_4$	13A-6	143
		13A-4	141

V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
AsH <sub>6</sub> NO <sub>4</sub>	NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	13A-8	147
AsH <sub>2</sub> O <sub>4</sub> Rb	RbH <sub>2</sub> AsO <sub>4</sub>	13A-5	143
Azobenzene	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub>	37-5	216
Azoxybenzene	C <sub>12</sub> H <sub>10</sub> N <sub>2</sub> O	37-6	216
B <sub>7</sub> BrCd <sub>3</sub> O <sub>13</sub>	Cd <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-18	120
B <sub>7</sub> BrCo <sub>3</sub> O <sub>13</sub>	Co <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-14	119
B <sub>7</sub> BrCr <sub>3</sub> O <sub>13</sub>	Cr <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-11	118
B <sub>7</sub> BrCu <sub>3</sub> O <sub>13</sub>	Cu <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-16	119
B <sub>7</sub> BrFe <sub>3</sub> O <sub>13</sub>	Fe <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-13	119
B <sub>7</sub> BrMg <sub>3</sub> O <sub>13</sub>	Mg <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-10	118
B <sub>7</sub> BrMn <sub>3</sub> O <sub>13</sub>	Mn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-12	119
B <sub>7</sub> BrNi <sub>3</sub> O <sub>13</sub>	Ni <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-15	119
B <sub>7</sub> BrO <sub>13</sub> Zn <sub>3</sub>	Zn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Br	9A-17	120
B <sub>6</sub> Ca <sub>2</sub> H <sub>10</sub> O <sub>16</sub>	Ca <sub>2</sub> B <sub>6</sub> O <sub>11</sub> · 5H <sub>2</sub> O	21A-1	173
B <sub>6</sub> Ca <sub>2</sub> O <sub>11</sub> · 5H <sub>2</sub> O	Ca <sub>2</sub> B <sub>6</sub> O <sub>11</sub> · 5H <sub>2</sub> O	21A-1	173
B <sub>7</sub> Cd <sub>3</sub> ClO <sub>13</sub>	Cd <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-9	118
B <sub>7</sub> Cd <sub>3</sub> IO <sub>13</sub>	Cd <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-25	122
B <sub>7</sub> ClCo <sub>3</sub> O <sub>13</sub>	Co <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-5	117
B <sub>7</sub> ClCr <sub>3</sub> O <sub>13</sub>	Cr <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-2	116
B <sub>7</sub> ClCu <sub>3</sub> O <sub>13</sub>	Cu <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-7	118
B <sub>7</sub> ClFe <sub>3</sub> O <sub>13</sub>	Fe <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-4	117
B <sub>7</sub> ClMg <sub>3</sub> O <sub>13</sub>	Mg <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-1	115
B <sub>7</sub> ClMn <sub>3</sub> O <sub>13</sub>	Mn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-3	117
B <sub>7</sub> ClNi <sub>3</sub> O <sub>13</sub>	Ni <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-6	117
B <sub>7</sub> ClO <sub>13</sub> Zn <sub>3</sub>	Zn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> Cl	9A-8	118
B <sub>7</sub> Co <sub>3</sub> IO <sub>13</sub>	Co <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-22	121
B <sub>7</sub> Cr <sub>3</sub> IO <sub>13</sub>	Cr <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-19	120
B <sub>7</sub> Fe <sub>3</sub> IO <sub>13</sub>	Fe <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-21	120
B <sub>7</sub> IMn <sub>3</sub> O <sub>13</sub>	Mn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-20	120
B <sub>7</sub> INi <sub>3</sub> O <sub>13</sub>	Ni <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-23	121
B <sub>7</sub> IO <sub>13</sub> Zn <sub>3</sub>	Zn <sub>3</sub> B <sub>7</sub> O <sub>13</sub> I	9A-24	121
Ba <sub>4</sub> Bi <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	Ba <sub>4</sub> Bi <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-g1	104
BaBi <sub>2</sub> Nb <sub>8</sub> O <sub>9</sub>	BaBi <sub>2</sub> Nb <sub>8</sub> O <sub>9</sub>	7A-7	109
BaBi <sub>3</sub> NbO <sub>12</sub> Ti <sub>2</sub>	BaBi <sub>3</sub> Ti <sub>2</sub> NbO <sub>12</sub>	7A-12	110
BaBi <sub>2</sub> O <sub>9</sub> Ta <sub>2</sub>	BaBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub>	7A-8	109
BaBi <sub>4</sub> O <sub>15</sub> Ti <sub>4</sub>	BaBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub>	7A-14	111
Ba <sub>2</sub> Bi <sub>4</sub> O <sub>18</sub> Ti <sub>5</sub>	Ba <sub>2</sub> Bi <sub>4</sub> Ti <sub>5</sub> O <sub>18</sub>	7A-19	112
BaC <sub>18</sub> Ca <sub>2</sub> H <sub>30</sub> O <sub>12</sub>	Ca <sub>2</sub> Ba(CH <sub>3</sub> CH <sub>2</sub> COO) <sub>6</sub>	26A-3	184
Ba <sub>4</sub> Ce <sub>2</sub> Nb <sub>8</sub> Ni <sub>2</sub> O <sub>30</sub>	Ba <sub>4</sub> Ce <sub>2</sub> Ni <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-d1	104
Ba <sub>4</sub> Fe <sub>2</sub> Gd <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	Ba <sub>4</sub> Gd <sub>2</sub> Fe <sub>2</sub> NbO <sub>30</sub>	5C-g4	104
Ba <sub>2</sub> Fe <sub>3</sub> Nb <sub>7</sub> Nd <sub>4</sub> O <sub>30</sub>	Ba <sub>2</sub> Nd <sub>4</sub> Fe <sub>3</sub> Nb <sub>7</sub> O <sub>30</sub>	5C-h1	104
Ba <sub>4</sub> Fe <sub>2</sub> Nb <sub>8</sub> Nd <sub>2</sub> O <sub>30</sub>	Ba <sub>4</sub> Nd <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-g2	104
Ba <sub>6</sub> FeNb <sub>9</sub> O <sub>30</sub>	Ba <sub>6</sub> FeNb <sub>9</sub> O <sub>30</sub>	5C-f1	104
Ba <sub>2</sub> Fe <sub>4</sub> Nb <sub>7</sub> O <sub>30</sub> Sm <sub>4</sub>	Ba <sub>2</sub> Sm <sub>4</sub> Fe <sub>4</sub> Nb <sub>7</sub> O <sub>30</sub>	5C-h2	104
Ba <sub>4</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub> Sm <sub>2</sub>	Ba <sub>4</sub> Sm <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-g3	104
Ba <sub>2</sub> KNb <sub>5</sub> O <sub>15</sub>	KBa <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	5C-b3	103
Ba <sub>9</sub> MgNb <sub>14</sub> O <sub>45</sub>	Ba <sub>9</sub> MgNb <sub>14</sub> O <sub>45</sub>	5C-e1	104
Ba <sub>2</sub> NaNb <sub>5</sub> O <sub>15</sub>	NaBa <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	5C-b2	103
Ba <sub>2</sub> Nb <sub>8</sub> Nd <sub>4</sub> Ni <sub>2</sub> O <sub>30</sub>	Ba <sub>2</sub> Nd <sub>4</sub> Ni <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-c1	104
Ba <sub>2</sub> Nb <sub>8</sub> Ni <sub>2</sub> O <sub>30</sub> Sm <sub>4</sub>	Ba <sub>2</sub> Sm <sub>4</sub> Ni <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-c2	104
Ba <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub> Rb	RbBa <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	5C-b5	103
Ba <sub>6</sub> Nb <sub>8</sub> O <sub>30</sub> Ti <sub>2</sub>	Ba <sub>6</sub> Ti <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-j1	104
BaNb <sub>1.5</sub> O <sub>5.25</sub> Zr <sub>0.25</sub>	BaZr <sub>0.25</sub> Nb <sub>1.5</sub> O <sub>5.25</sub>	5C-j3	105
BaO <sub>6</sub> Ta <sub>2</sub>	BaTa <sub>2</sub> O <sub>6</sub>	5A-3	98
BaO <sub>9</sub> Ti	BaTiO <sub>3</sub>	1A-8	51
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub>	1A-12	61
BeC <sub>6</sub> F <sub>4</sub> H <sub>17</sub> N <sub>2</sub> O <sub>6</sub>	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>4</sub> H <sub>2</sub> BeF <sub>4</sub>	28A-3	190
BeF <sub>4</sub> H <sub>8</sub> N <sub>2</sub>	(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub>	14A-2	154
BiBrS	BiSBr	10A-7	126
BiBrSe	BiSeBr	10A-10	127
Bi <sub>4</sub> CaNb <sub>2</sub> O <sub>9</sub>	CaBi <sub>4</sub> Nb <sub>2</sub> O <sub>9</sub>	7A-3	107
Bi <sub>2</sub> CaO <sub>9</sub> Ta <sub>2</sub>	CaBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub>	7A-4	108
Bi <sub>4</sub> CaO <sub>15</sub> Ti <sub>4</sub>	CaBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub>	7A-17	112

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Gross formula	Chemical formula	Nr.	Page
BiClS	BiS <sub>Cl</sub>	10A-6	125
BiClSe	BiSeCl	10A-9	126
Bi <sub>2</sub> Fe <sub>4</sub> Nb <sub>6</sub> Nd <sub>4</sub> O <sub>30</sub>	Bi <sub>2</sub> Nd <sub>4</sub> Fe <sub>4</sub> Nb <sub>6</sub> O <sub>30</sub>	5C-i2	104
BiFeO <sub>3</sub>	BiFeO <sub>3</sub>	1A-15	63
Bi <sub>5</sub> GaO <sub>15</sub> Ti <sub>3</sub>	BiBi <sub>4</sub> Ti <sub>3</sub> GaO <sub>15</sub>	7A-18	112
BiS	BiSI	10A-8	126
BiSe	BiSeI	10A-11	127
BiK <sub>2</sub> Nb <sub>6</sub> O <sub>15</sub>	K <sub>2</sub> BiNb <sub>6</sub> O <sub>15</sub>	5C-a2	102
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Ti	(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1B1-i	64
Bi <sub>4.5</sub> O <sub>15</sub> Ti <sub>4</sub>	K <sub>0.5</sub> Bi <sub>4.5</sub> Ti <sub>4</sub> O <sub>15</sub>	7B-4	114
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1B1-ii	64
Bi <sub>4.5</sub> Na <sub>0.5</sub> O <sub>15</sub> Ti <sub>4</sub>	Na <sub>0.5</sub> Bi <sub>4.5</sub> Ti <sub>4</sub> O <sub>15</sub>	7B-3	114
Bi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> Pb	PbBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	7A-9	109
Bi <sub>3</sub> NbO <sub>12</sub> PbTi <sub>2</sub>	PbBi <sub>3</sub> Ti <sub>2</sub> NbO <sub>12</sub>	7A-13	110
Bi <sub>4</sub> Nb <sub>2</sub> O <sub>9</sub> Sr	SrBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	7A-5	108
Bi <sub>3</sub> NbO <sub>9</sub> Ti	BiBi <sub>2</sub> TiNbO <sub>9</sub>	7A-1	107
Bi <sub>2</sub> O <sub>9</sub> PbTa <sub>2</sub>	PbBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub>	7A-10	110
Bi <sub>4</sub> O <sub>15</sub> PbTi <sub>4</sub>	PbBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub>	7A-15	111
Bi <sub>4</sub> O <sub>15</sub> Pb <sub>2</sub> Ti <sub>5</sub>	Pb <sub>2</sub> Bi <sub>4</sub> Ti <sub>5</sub> O <sub>18</sub>	7A-20	112
Bi <sub>2</sub> O <sub>9</sub> SrTa <sub>2</sub>	SrBi <sub>2</sub> Ta <sub>2</sub> O <sub>9</sub>	7A-6	109
Bi <sub>4</sub> O <sub>15</sub> SrTi <sub>4</sub>	SrBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub>	7A-16	111
Bi <sub>4</sub> O <sub>18</sub> Sr <sub>2</sub> Ti <sub>5</sub>	Sr <sub>2</sub> Bi <sub>4</sub> Ti <sub>5</sub> O <sub>18</sub>	7A-21	113
Bi <sub>3</sub> O <sub>9</sub> TaTi	BiBi <sub>2</sub> TiTaO <sub>9</sub>	7A-2	107
Bi <sub>2</sub> O <sub>11</sub> Ti <sub>4</sub>	Bi <sub>2</sub> Ti <sub>4</sub> O <sub>11</sub>	7A-22	113
Bi <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub>	BiBi <sub>3</sub> Ti <sub>2</sub> TiO <sub>12</sub>	7A-11	110
Br <sub>3</sub> C <sub>4</sub> H <sub>12</sub> HgN	N(CH <sub>3</sub> ) <sub>4</sub> HgBr <sub>3</sub>	24A-2	179
Br <sub>3</sub> C <sub>4</sub> H <sub>12</sub> HgP	P(CH <sub>3</sub> ) <sub>4</sub> HgBr <sub>3</sub>	24A-3	180
BrH	H · Br	35-12	203
BrSSb	SbSBr	10A-1	122
BrSbSe	SbSeBr	10A-3	124
C <sub>9</sub> CaCl <sub>2</sub> H <sub>21</sub> N <sub>3</sub> O <sub>6</sub>	(CH <sub>3</sub> NHCH <sub>2</sub> COOH) <sub>3</sub> · CaCl <sub>2</sub>	32A-1	192
C <sub>18</sub> Ca <sub>2</sub> H <sub>30</sub> O <sub>12</sub> Pb	Ca <sub>2</sub> Pb(CH <sub>3</sub> CH <sub>2</sub> COO) <sub>6</sub>	26A-2	183
C <sub>18</sub> Ca <sub>2</sub> H <sub>30</sub> O <sub>12</sub> Sr	Ca <sub>2</sub> Sr(CH <sub>3</sub> CH <sub>2</sub> COO) <sub>6</sub>	26A-1	182
C <sub>4</sub> Cl <sub>3</sub> H <sub>12</sub> HgN	N(CH <sub>3</sub> ) <sub>4</sub> · HgCl <sub>3</sub>	24A-1	178
C <sub>4</sub> Cl <sub>4</sub> H <sub>10</sub> MnN <sub>3</sub> O <sub>4</sub> · 2H <sub>2</sub> O	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>2</sub> · MnCl <sub>2</sub> · 2H <sub>2</sub> O	31A-1	192
C <sub>4</sub> Cl <sub>2</sub> H <sub>14</sub> MnN <sub>3</sub> O <sub>6</sub>	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>2</sub> · MnCl <sub>2</sub> · 2H <sub>2</sub> O	31A-1	192
C <sub>2</sub> ClH <sub>6</sub> NO <sub>2</sub>	CH <sub>2</sub> ClCOONH <sub>4</sub>	27A-1	184
C <sub>4</sub> Cl <sub>2</sub> H <sub>6</sub> NO <sub>4</sub>	(CH <sub>2</sub> ClCOO) <sub>2</sub> · NH <sub>4</sub>	27A-2	184
CCrH <sub>6</sub> NO <sub>6</sub> S <sub>2</sub> · 12H <sub>2</sub> O	CH <sub>3</sub> NH <sub>3</sub> Cr(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-6	160
CCrH <sub>6</sub> N <sub>3</sub> O <sub>8</sub> S <sub>2</sub> · 6H <sub>2</sub> O	C(NH <sub>2</sub> ) <sub>3</sub> Cr(SO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-2	164
CCrH <sub>30</sub> NO <sub>20</sub> S <sub>2</sub>	CH <sub>3</sub> NH <sub>3</sub> Cr(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-6	160
CCrH <sub>18</sub> N <sub>3</sub> O <sub>14</sub> S <sub>2</sub>	C(NH <sub>2</sub> ) <sub>3</sub> Cr(SO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-2	164
CCrH <sub>6</sub> N <sub>3</sub> O <sub>8</sub> Se <sub>2</sub> · 6H <sub>2</sub> O	C(NH <sub>2</sub> ) <sub>3</sub> Cr(SeO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-6	167
CCrH <sub>18</sub> N <sub>3</sub> O <sub>14</sub> Se <sub>2</sub>	C(NH <sub>2</sub> ) <sub>3</sub> Cr(SeO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-6	167
C <sub>2</sub> CuH <sub>2</sub> O <sub>4</sub> · 4H <sub>2</sub> O	Cu(HCOO) <sub>2</sub> · 4H <sub>2</sub> O	19A-6	167
C <sub>2</sub> CuH <sub>10</sub> O <sub>8</sub>	Cu(HCOO) <sub>2</sub> · 4H <sub>2</sub> O	25A-1	180
C <sub>6</sub> FeH <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	25A-1	180
CFeH <sub>6</sub> NO <sub>8</sub> S <sub>2</sub> · 12H <sub>2</sub> O	CH <sub>3</sub> NH <sub>3</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	22A-2	174
CFeH <sub>30</sub> NO <sub>20</sub> S <sub>2</sub>	CH <sub>3</sub> NH <sub>3</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-7	160
C <sub>9</sub> FeK <sub>4</sub> N <sub>6</sub> · 3H <sub>2</sub> O	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	18A-7	160
CGaH <sub>6</sub> NO <sub>8</sub> S <sub>2</sub> · 12H <sub>2</sub> O	CH <sub>3</sub> NH <sub>3</sub> Ga(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	22A-2	174
CGaH <sub>6</sub> N <sub>3</sub> O <sub>8</sub> S <sub>2</sub> · 6H <sub>2</sub> O	C(NH <sub>2</sub> ) <sub>3</sub> Ga(SO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	18A-5	160
CGaH <sub>18</sub> N <sub>3</sub> O <sub>14</sub> S <sub>2</sub>	C(NH <sub>2</sub> ) <sub>3</sub> Ga(SO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-3	165
CGaH <sub>30</sub> NO <sub>20</sub> S <sub>2</sub>	CH <sub>3</sub> NH <sub>3</sub> Ga(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	19A-3	165
CGaH <sub>6</sub> N <sub>3</sub> O <sub>8</sub> Se <sub>2</sub> · 6H <sub>2</sub> O	C(NH <sub>2</sub> ) <sub>3</sub> Ga(SeO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	18A-5	160
CGaH <sub>18</sub> N <sub>3</sub> O <sub>14</sub> Se <sub>2</sub>	C(NH <sub>2</sub> ) <sub>3</sub> Ga(SeO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-7	167
C <sub>4</sub> H <sub>12</sub> HgI <sub>3</sub> N	N(CH <sub>3</sub> ) <sub>4</sub> HgI <sub>3</sub>	19A-7	167
C <sub>6</sub> H <sub>6</sub> K <sub>4</sub> MnN <sub>6</sub> O <sub>3</sub>	K <sub>4</sub> Mn(CN) <sub>6</sub> · 3H <sub>2</sub> O	24A-4	180
C <sub>6</sub> H <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub> Os	K <sub>4</sub> Os(CN) <sub>6</sub> · 3H <sub>2</sub> O	22A-1	174
C <sub>6</sub> H <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub> Ru	K <sub>4</sub> Ru(CN) <sub>6</sub> · 3H <sub>2</sub> O	22A-4	176
C <sub>4</sub> H <sub>4</sub> KNaO <sub>6</sub> · 4H <sub>2</sub> O	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	22A-3	176
C <sub>4</sub> H <sub>12</sub> KNaO <sub>10</sub>	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-1	193
C <sub>4</sub> H <sub>8</sub> LiNO <sub>6</sub> · H <sub>2</sub> O	LiNH <sub>4</sub> · C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · H <sub>2</sub> O	33A-1	193
		34A-1	199

V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
C <sub>4</sub> H <sub>10</sub> LiNO <sub>7</sub>	LiNH <sub>4</sub> · C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · H <sub>2</sub> O	34A-1	199
C <sub>4</sub> H <sub>4</sub> LiO <sub>6</sub> Tl · H <sub>2</sub> O	LiTiC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · H <sub>2</sub> O	34A-2	199
C <sub>4</sub> H <sub>6</sub> LiO <sub>7</sub> Tl	LiTiC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · H <sub>2</sub> O	34A-2	199
C <sub>4</sub> H <sub>8</sub> NNaO <sub>6</sub> · 4H <sub>2</sub> O	NaNH <sub>4</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-2	197
C <sub>4</sub> H <sub>16</sub> NNaO <sub>10</sub>	NaNH <sub>4</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-2	197
C <sub>4</sub> H <sub>11</sub> N <sub>3</sub> O <sub>7</sub>	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>2</sub> · HNO <sub>3</sub>	30A-1	191
C <sub>6</sub> H <sub>17</sub> N <sub>3</sub> O <sub>10</sub> S	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SO <sub>4</sub>	28A-1	185
CH <sub>6</sub> NO <sub>8</sub> S <sub>2</sub> V · 12H <sub>2</sub> O	CH <sub>3</sub> NH <sub>3</sub> V(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-8	161
CH <sub>6</sub> N <sub>3</sub> O <sub>5</sub> S <sub>2</sub> V · 6H <sub>2</sub> O	C(NH <sub>2</sub> ) <sub>3</sub> V(SO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-4	166
CH <sub>16</sub> N <sub>3</sub> O <sub>14</sub> S <sub>2</sub> V	C(NH <sub>2</sub> ) <sub>3</sub> V(SO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-4	166
CH <sub>30</sub> NO <sub>20</sub> S <sub>2</sub> V	CH <sub>3</sub> NH <sub>3</sub> V(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-8	161
C <sub>6</sub> H <sub>17</sub> N <sub>3</sub> O <sub>10</sub> Se	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SeO <sub>4</sub>	28A-2	190
CH <sub>4</sub> N <sub>2</sub> S	SC(NH <sub>2</sub> ) <sub>2</sub>	23A-1	177
C <sub>4</sub> H <sub>4</sub> NaO <sub>6</sub> Rb · 4H <sub>2</sub> O	NaRbC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-3	198
C <sub>4</sub> H <sub>12</sub> NaO <sub>10</sub> Rb	NaRbC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-3	198
CH <sub>6</sub> InNO <sub>8</sub> S <sub>2</sub> · 12H <sub>2</sub> O	CH <sub>3</sub> NH <sub>3</sub> In(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-9	161
CH <sub>30</sub> InNO <sub>20</sub> S <sub>2</sub>	CH <sub>3</sub> NH <sub>3</sub> In(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-9	161
C <sub>6</sub> K <sub>4</sub> MnN <sub>6</sub> · 3H <sub>2</sub> O	K <sub>4</sub> Mn(CN) <sub>6</sub> · 3H <sub>2</sub> O	22A-1	174
C <sub>6</sub> K <sub>4</sub> N <sub>6</sub> Os · 3H <sub>2</sub> O	K <sub>4</sub> Os(CN) <sub>6</sub> · 3H <sub>2</sub> O	22A-4	176
C <sub>6</sub> K <sub>4</sub> N <sub>6</sub> Ru · 3H <sub>2</sub> O	K <sub>4</sub> Ru(CN) <sub>6</sub> · 3H <sub>2</sub> O	22A-3	176
CaO <sub>3</sub> Ti	CaTiO <sub>3</sub>	1A-5	44
CaO <sub>3</sub> Zr	CaZrO <sub>3</sub>	1A-10	60
Cd <sub>2</sub> H <sub>8</sub> N <sub>2</sub> O <sub>12</sub> S <sub>3</sub>	(NH <sub>4</sub> ) <sub>2</sub> Cd <sub>2</sub> (SO <sub>4</sub> ) <sub>3</sub>	16A-1	156
Cd <sub>1/4</sub> Mn <sub>1/4</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Cd <sub>1/4</sub> Mn <sub>1/4</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
Cd <sub>1/4</sub> Mn <sub>1/4</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Cd <sub>1/4</sub> Mn <sub>1/4</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6A-1	105
Cd <sub>1/3</sub> Nb <sub>2/3</sub> O <sub>3</sub> Pb	Pb(Cd <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1B4-iii	71
Cd <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Cd <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B2-ii	65
CdO <sub>3</sub> Ti	CdTiO <sub>3</sub>	1A-7	50
Cl <sub>3</sub> CsGe	CsGeCl <sub>3</sub>	35-21	208
ClH	HCl	35-11	202
CIK	KCl	35-28	211
CoCrH <sub>5</sub> N <sub>3</sub> O <sub>8</sub> S <sub>2</sub> · 12H <sub>2</sub> O	Co(NH <sub>2</sub> ) <sub>2</sub> HCr(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-11	161
CoCrH <sub>29</sub> N <sub>2</sub> O <sub>20</sub> S <sub>2</sub>	Co(NH <sub>2</sub> ) <sub>2</sub> HCr(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-11	161
Colemanite	Ca <sub>2</sub> B <sub>6</sub> O <sub>11</sub> · 5H <sub>2</sub> O or CaB <sub>3</sub> O <sub>4</sub> (OH) <sub>3</sub> · H <sub>2</sub> O	21A-1	173
Co <sub>1/4</sub> Mn <sub>1/4</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Co <sub>1/4</sub> Mn <sub>1/4</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
Co <sub>1/4</sub> Mn <sub>1/4</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Co <sub>1/4</sub> Mn <sub>1/4</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
Co <sub>1/3</sub> Nb <sub>2/3</sub> O <sub>3</sub> Pb	Pb(Co <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1B4-iv	71
Co <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Co <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-iv	68
Co <sub>1/3</sub> O <sub>3</sub> PbTa <sub>2/3</sub>	Pb(Co <sub>1/3</sub> Ta <sub>2/3</sub> )O <sub>3</sub>	1B4-vii	72
Co <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Co <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-xiii	70
Co <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Co <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B2-iv	66
Cr <sub>1/4</sub> Nb <sub>1/2</sub> O <sub>3</sub> PbSc <sub>1/4</sub>	Pb(Sc <sub>1/4</sub> Cr <sub>1/4</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
CsH <sub>2</sub> O <sub>4</sub> P	CsH <sub>2</sub> PO <sub>4</sub>	13A-3	141
CsH <sub>3</sub> O <sub>6</sub> Se <sub>2</sub>	CsH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub>	20A-3	172
CsNO <sub>3</sub>	CsNO <sub>3</sub>	12A-3	134
Deoxyribonucleic acid	Deoxyribonucleic acid	35-33	212
DNA	Deoxyribonucleic acid	35-33	212
ErMnO <sub>3</sub>	ErMnO <sub>3</sub>	4A-2	95
Eu <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	Eu <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-2	200
F <sub>7</sub> H <sub>8</sub> N <sub>2</sub> P	NH <sub>4</sub> PF <sub>6</sub> NH <sub>4</sub> F	35-24	210
FeH <sub>4</sub> NO <sub>8</sub> S <sub>2</sub> · 12H <sub>2</sub> O	NH <sub>4</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-1	157
FeH <sub>28</sub> NO <sub>20</sub> S <sub>2</sub>	NH <sub>4</sub> Fe(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-1	157
Fe <sub>4</sub> Nb <sub>6</sub> Nd <sub>6</sub> O <sub>30</sub>	Nd <sub>6</sub> Fe <sub>4</sub> Nb <sub>6</sub> O <sub>30</sub>	5C-i1	104
Fe <sub>3</sub> Nb <sub>7</sub> Nd <sub>4</sub> O <sub>30</sub> Pb <sub>2</sub>	Pb <sub>2</sub> Nd <sub>4</sub> Fe <sub>3</sub> Nb <sub>7</sub> O <sub>30</sub>	5C-h3	104
Fe <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-iii	67
FeNb <sub>9</sub> O <sub>30</sub> Sr <sub>6</sub>	Sr <sub>6</sub> FeNb <sub>9</sub> O <sub>30</sub>	5C-f2	104
Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub> Sr <sub>4</sub> Yb <sub>2</sub>	Sr <sub>4</sub> Yb <sub>2</sub> Fe <sub>2</sub> Nb <sub>8</sub> O <sub>30</sub>	5C-g5	104
Fe <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-xii	69
Fe <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Fe <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B3-xvi	70
Fe <sub>2/3</sub> O <sub>3</sub> PbW <sub>1/3</sub>	Pb(Fe <sub>2/3</sub> W <sub>1/3</sub> )O <sub>3</sub>	1B5-ii	73

GA  
Gd<sub>2</sub>  
Ge<sub>3</sub>

HI  
H<sub>11</sub>  
H<sub>4</sub>  
H<sub>2</sub>  
H<sub>6</sub>  
H<sub>3</sub>  
H<sub>4</sub>  
H<sub>5</sub>

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199	GASH	C(NH <sub>2</sub> ) <sub>3</sub> Al(SO <sub>4</sub> ) <sub>2</sub> · 6H <sub>2</sub> O	19A-1	161
199	Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	Gd <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-3	200
199	GeTe	GeTe	36-1	212
197	HI	HI		
191	H <sub>11</sub> InN <sub>2</sub> O <sub>6</sub>	(NH <sub>4</sub> ) <sub>2</sub> H <sub>3</sub> IO <sub>6</sub>	35-13	204
185	H <sub>4</sub> InNO <sub>8</sub> S <sub>2</sub> · 12H <sub>2</sub> O	NH <sub>4</sub> In(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	35-23	209
161	H <sub>28</sub> InNO <sub>20</sub> S <sub>2</sub>	NH <sub>4</sub> In(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-3	158
166	H <sub>4</sub> KO <sub>4</sub> P	KH <sub>2</sub> PO <sub>4</sub>	18A-3	158
166	H <sub>4</sub> LiN <sub>2</sub> O <sub>4</sub> S	Li(N <sub>2</sub> H <sub>5</sub> )SO <sub>4</sub>	13A-1	134
161	H <sub>3</sub> LiO <sub>6</sub> Se <sub>2</sub>	LiH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub>	35-15	205
190	H <sub>4</sub> NNaO <sub>4</sub> S · 2H <sub>2</sub> O	NaNH <sub>4</sub> SO <sub>4</sub> · 2H <sub>2</sub> O	20A-1	168
177	H <sub>6</sub> NNaO <sub>6</sub> S	NaNH <sub>4</sub> SO <sub>4</sub> · 2H <sub>2</sub> O	17A-1	157
198	H <sub>6</sub> NO <sub>4</sub> P	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	17A-1	157
198	H <sub>5</sub> NO <sub>4</sub> S	(NH <sub>4</sub> )HSO <sub>4</sub>	13A-7	143
161	H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> S	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	15A-1	154
161	H <sub>4</sub> NO <sub>8</sub> S <sub>2</sub> V · 12H <sub>2</sub> O	NH <sub>4</sub> V(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	14A-1	148
174	H <sub>28</sub> NO <sub>20</sub> S <sub>2</sub> V	NH <sub>4</sub> V(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O	18A-2	158
176	H <sub>3</sub> NaO <sub>6</sub> Se <sub>2</sub>	NaH <sub>3</sub> (SeO <sub>3</sub> ) <sub>2</sub>	18A-2	158
176	H <sub>2</sub> O (Ice)	H <sub>2</sub> O	20A-2	169
44	H <sub>2</sub> O <sub>4</sub> PRb	RbH <sub>2</sub> PO <sub>4</sub>	35-29	211
60	HO <sub>4</sub> RbS	RbHSO <sub>4</sub>	13A-2	141
156	HfO <sub>3</sub> Pb	PbHfO <sub>3</sub>	15A-2	155
70	HoMnO <sub>3</sub>	HoMnO <sub>3</sub>	1A-14	62
70	Ho <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Ho <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	4A-3	95
105			1B3-viii	68
71	Ice	H <sub>2</sub> O		
65	IKO <sub>3</sub>	KIO <sub>3</sub>	35-29	211
50	ISSb	SbSI	1A-16	64
208	ISbSe	SbSeI	10A-2	122
202	ISbTe	SbTeI	10A-4	125
211	In <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(In <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	10A-5	125
161			1B3-vi	68
161	KDP	KH <sub>2</sub> PO <sub>4</sub>		
173	K <sub>2</sub> LaNb <sub>5</sub> O <sub>15</sub>	K <sub>2</sub> LaNb <sub>5</sub> O <sub>15</sub>	13A-1	134
70	K <sub>0.6</sub> Li <sub>0.4</sub> NbO <sub>3</sub>	K <sub>0.6</sub> Li <sub>0.4</sub> NbO <sub>3</sub>	5C-a1	102
70	K <sub>0.6</sub> Li <sub>0.4</sub> Nb <sub>0.3</sub> O <sub>3</sub> Ta <sub>0.7</sub>	K <sub>0.6</sub> Li <sub>0.4</sub> (Ta <sub>0.7</sub> Nb <sub>0.3</sub> )O <sub>3</sub>	5C-k1	105
71	KLiO <sub>4</sub> S	KLiSO <sub>4</sub>	5C-k2	105
68	KNO <sub>2</sub>	KNO <sub>2</sub>	35-27	211
72	KNO <sub>3</sub>	KNO <sub>3</sub>	11A-2	130
70	KNbO <sub>3</sub>	KNbO <sub>3</sub>	12A-1	131
66	KNb <sub>5</sub> O <sub>15</sub> Sr <sub>2</sub>	KSr <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	1A-2	39
70	KO <sub>3</sub> Ta	KTaO <sub>3</sub>	5C-b1	102
141			1A-4	41
172	Lecontite	NaNH <sub>4</sub> SO <sub>4</sub> · 2H <sub>2</sub> O		
134	LiNbO <sub>3</sub>	LiNbO <sub>3</sub>	17A-1	157
	Li <sub>1/4</sub> Nb <sub>1/4</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Li <sub>1/4</sub> Nb <sub>1/4</sub> W <sub>1/2</sub> )O <sub>3</sub>	3A-1	89
212	LiO <sub>3</sub> Ta	LiTaO <sub>3</sub>	1B3-xvii	70
212	LuMnO <sub>3</sub>	LuMnO <sub>3</sub>	3A-2	92
95	Lu <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Lu <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	4A-6	97
200	Lu <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Lu <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-ix	68
			1B3-xv	70
210	MASD	CH <sub>3</sub> NH <sub>3</sub> Al(SO <sub>4</sub> ) <sub>2</sub> · 12H <sub>2</sub> O		
157	Mg <sub>1/4</sub> Mn <sub>1/4</sub> Nb <sub>1/4</sub> O <sub>3</sub> Pb	Pb(Mg <sub>1/4</sub> Mn <sub>1/4</sub> Nb <sub>1/4</sub> )O <sub>3</sub>	18A-4	158
157	Mg <sub>1/4</sub> Mn <sub>1/4</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Mg <sub>1/4</sub> Mn <sub>1/4</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
104	Mg <sub>1/4</sub> Mn <sub>1/4</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Mg <sub>1/4</sub> Mn <sub>1/4</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
104	Mg <sub>1/3</sub> Nb <sub>2/3</sub> O <sub>3</sub> Pb	Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1B3-xvii	70
67	MgNb <sub>14</sub> O <sub>45</sub> Sr <sub>9</sub>	Sr <sub>9</sub> MgNb <sub>14</sub> O <sub>45</sub>	1B4-i	70
104	Mg <sub>1/3</sub> O <sub>3</sub> PbTa <sub>2/3</sub>	Pb(Mg <sub>1/3</sub> Ta <sub>2/3</sub> )O <sub>3</sub>	5C-e2	104
104	Mg <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B4-vi	72
69	Mn <sub>1/4</sub> Nb <sub>1/2</sub> Ni <sub>1/4</sub> O <sub>3</sub> Pb	Pb(Ni <sub>1/4</sub> Mn <sub>1/4</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B2-i	65
70	Mn <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Mn <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
73	Mn <sub>1/4</sub> Nb <sub>1/2</sub> O <sub>3</sub> PbZn <sub>1/4</sub>	Pb(Zn <sub>1/4</sub> Mn <sub>1/4</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-ii	67
	Mn <sub>1/4</sub> Ni <sub>1/4</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Ni <sub>1/4</sub> Mn <sub>1/4</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B3-xvii	70
			1B3-xvii	70

V Substanzenverzeichnis

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MnO <sub>2</sub>	MnO <sub>2</sub>	35-31	212
Mn <sub>1/2</sub> O <sub>3</sub> PbRe <sub>1/2</sub>	Pb(Mn <sub>1/2</sub> Re <sub>1/2</sub> )O <sub>3</sub>	1B2-v	66
Mn <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Mn <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-xi	69
Mn <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Mn <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1B2-iii	66
Mn <sub>2/3</sub> O <sub>3</sub> PbW <sub>1/3</sub>	Pb(Mn <sub>2/3</sub> W <sub>1/3</sub> )O <sub>3</sub>	1B5-i	73
MnO <sub>3</sub> Tm	TmMnO <sub>3</sub>	4A-4	96
MnO <sub>3</sub> Y	YMnO <sub>3</sub>	4A-1	94
MnO <sub>3</sub> Yb	YbMnO <sub>3</sub>	4A-5	96
Mo <sub>3</sub> O <sub>12</sub> Sm <sub>2</sub>	Sm <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-1	200
Mo <sub>3</sub> O <sub>12</sub> Tb <sub>2</sub>	Tb <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-4	201
NNaO <sub>2</sub>	NaNO <sub>2</sub>	11A-1	128
NO <sub>3</sub> Rb	RbNO <sub>3</sub>	12A-2	133
NaNbO <sub>3</sub>	NaNbO <sub>3</sub>	1A-1	37
NaO <sub>3</sub> Ta	NaTaO <sub>3</sub>	1A-3	40
NaO <sub>3</sub> V	NaVO <sub>3</sub>	35-19	208
Nb <sub>1/2</sub> Ni <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Ni <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-v	68
Nb <sub>2/3</sub> Ni <sub>1/3</sub> O <sub>3</sub> Pb	Pb(Ni <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1B4-v	72
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub>	5A-1	97
Nb <sub>2</sub> O <sub>6</sub> Pb <sub>2</sub>	Pb <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6A-2	106
Nb <sub>1/2</sub> O <sub>3</sub> PbSc <sub>1/2</sub>	Pb(Sc <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-i	67
Nb <sub>1/2</sub> O <sub>3</sub> PbYb <sub>1/2</sub>	Pb(Yb <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1B3-vii	68
Nb <sub>2/3</sub> O <sub>3</sub> PbZn <sub>1/3</sub>	Pb(Zn <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub>	1B4-ii	71
Nb <sub>5</sub> O <sub>15</sub> RbSr <sub>2</sub>	RbSr <sub>2</sub> Nb <sub>5</sub> O <sub>15</sub>	5C-b4	103
Ni <sub>1/3</sub> O <sub>3</sub> PbTa <sub>2/3</sub>	Pb(Ni <sub>1/3</sub> Ta <sub>2/3</sub> )O <sub>3</sub>	1B4-viii	73
O <sub>3</sub> PbSc <sub>1/2</sub> Ta <sub>1/2</sub>	Pb(Sc <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-x	69
O <sub>6</sub> Pb <sub>4</sub> Si	Pb <sub>4</sub> SiO <sub>6</sub>	35-26	210
O <sub>6</sub> PbTa <sub>2</sub>	PbTa <sub>2</sub> O <sub>6</sub>	5A-4	98
O <sub>3</sub> PbTa <sub>1/3</sub> Yb <sub>1/2</sub>	Pb(Yb <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1B3-xiv	70
O <sub>3</sub> PbTi	PbTiO <sub>3</sub>	1A-9	59
O <sub>6</sub> Pb <sub>2</sub> V <sub>2</sub>	Pb <sub>2</sub> V <sub>2</sub> O <sub>8</sub>	35-25	210
O <sub>3</sub> PbZr	PbZrO <sub>3</sub>	1A-13	61
O <sub>3</sub> RbTa	RbTaO <sub>3</sub>	35-17	207
O <sub>2</sub> Sn	SnO <sub>2</sub>	35-32	212
O <sub>4</sub> SrTa <sub>2</sub>	SrTa <sub>2</sub> O <sub>6</sub>	5A-2	98
O <sub>7</sub> Sr <sub>2</sub> Ta <sub>2</sub>	Sr <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	6A-3	106
O <sub>3</sub> SrTi	SrTiO <sub>3</sub>	1A-6	45
O <sub>3</sub> SrZr	SrZrO <sub>3</sub>	1A-11	61
O <sub>2</sub> Ti	TiO <sub>2</sub>	35-30	212
O <sub>3</sub> W	WO <sub>3</sub>	2A-1	88
p-azoxyanisole	C <sub>14</sub> H <sub>14</sub> N <sub>2</sub> O <sub>3</sub>	37-1	215
p-azoxypheonetole	C <sub>16</sub> H <sub>16</sub> N <sub>2</sub> O <sub>3</sub>	37-2	215
p-butoxybenzoic acid	C <sub>11</sub> H <sub>14</sub> O <sub>3</sub>	37-3	215
Perovskite	CaTiO <sub>3</sub>	1A-5	44
p-methoxycinnamic acid	C <sub>10</sub> H <sub>10</sub> O <sub>3</sub>	37-4	216
Pyrolusite	MnO <sub>2</sub>	35-31	212
Rochelle salt	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-1	193
RS	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-1	193
Rutile	TiO <sub>2</sub>	35-30	212
Seignette salt	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33A-1	193
SiV <sub>2</sub>	V <sub>2</sub> Si	36-4	214
SnTe	SnTe	36-2	213
TGS	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> H <sub>2</sub> SO <sub>4</sub>	28A-1	185
Tri-glycine tellurate		28A-4	190

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Al <sub>2</sub> BaO <sub>4</sub>	BaAl <sub>2</sub> O <sub>4</sub> -BaLi <sub>2</sub> F <sub>4</sub>	8B-1	115
AlLaO <sub>3</sub>	LaAlO <sub>3</sub> -BaTiO <sub>3</sub>	1C-c8	83
AlLaO <sub>3</sub>	LaAlO <sub>3</sub> -BiFeO <sub>3</sub>	1C-b11	83
AlLaO <sub>3</sub>	LaAlO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c10	84
AsH <sub>6</sub> NO <sub>4</sub>	NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub> -TH <sub>2</sub> AsO <sub>4</sub>	13B-3	148
AsH <sub>6</sub> O <sub>4</sub> Tl	TH <sub>2</sub> AsO <sub>4</sub> -NH <sub>4</sub> H <sub>2</sub> AsO <sub>4</sub>	13B-3	148
AsIS	AsSI-SbSI	10B-1	127
BaBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	(Ba-Pb)Bi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	7B-5	114
BaBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	Bi <sub>2</sub> BaNb <sub>2</sub> O <sub>9</sub> -Bi <sub>3</sub> TiNbO <sub>9</sub>	7B-1	113
BaBi <sub>3</sub> NbO <sub>12</sub> Ti <sub>2</sub>	Bi <sub>3</sub> BaTi <sub>2</sub> NbO <sub>12</sub> -Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub>	7B-2	113
BaF <sub>4</sub> Li <sub>2</sub>	BaLi <sub>4</sub> F <sub>4</sub> -BaAl <sub>2</sub> O <sub>4</sub>	8B-1	115
BaFe <sub>1/2</sub> O <sub>3</sub> Ta <sub>1/2</sub>	Ba(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> -BaTiO <sub>3</sub>	1C-d2	84
BaHfO <sub>3</sub>	BaHfO <sub>3</sub> -BaTiO <sub>3</sub>	1C-a24	77
BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -BaTiO <sub>3</sub>	1C-a18	76
BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -BaZrO <sub>3</sub>	1C-e9	86
BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -CaNb <sub>2</sub> O <sub>6</sub>	5C-j2	105
BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-1	99
BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -SrNb <sub>2</sub> O <sub>6</sub>	5B-5	100
BaNb <sub>2</sub> O <sub>6</sub>	BaNb <sub>2</sub> O <sub>6</sub> -BaTiO <sub>3</sub> -PbTiO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-3	99
BaNb <sub>2</sub> O <sub>6</sub>	(Ba-Pb-Sr)(Nb-Ta) <sub>2</sub> O <sub>6</sub>	1C-f19	88
BaNb <sub>2</sub> O <sub>6</sub>	(Ba-Pb-Ca)(Nb-Ta) <sub>2</sub> O <sub>6</sub>	5B-15	102
BaNb <sub>2</sub> O <sub>6</sub>	BaZr <sub>0.25</sub> Nb <sub>1.5</sub> O <sub>5.25</sub>	5B-15	102
BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -BaTiO <sub>3</sub>	5C-j3	105
BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-a25	77
BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a21	76
BaO <sub>3</sub> Sn	(Ba-Pb)(Sn-Ti)O <sub>3</sub>	1C-b10	83
BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -SrSnO <sub>3</sub>	1C-f18	88
BaO <sub>3</sub> Sn	BaSnO <sub>3</sub> -CaSnO <sub>3</sub> -SrSnO <sub>3</sub>	1C-a20	76
BaO <sub>6</sub> Ta <sub>2</sub>	BaTa <sub>2</sub> O <sub>6</sub> -BaTiO <sub>3</sub>	1C-f13	88
BaO <sub>6</sub> Ta <sub>2</sub>	(Ba-Pb-Ca)(Ta-Nb) <sub>2</sub> O <sub>6</sub>	1C-e10	87
BaO <sub>6</sub> Ta <sub>2</sub>	(Ba-Pb-Sr)(Ta-Nb) <sub>2</sub> O <sub>6</sub>	5B-15	102
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -Ba(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	5B-15	102
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -BaHfO <sub>3</sub>	1C-d2	84
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub>	1C-a24	77
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -BaSnO <sub>3</sub>	1C-e9	86
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -BaTa <sub>2</sub> O <sub>6</sub>	1C-a25	77
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -BaUC <sub>3</sub>	1C-e10	87
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -BaZrO <sub>3</sub>	1C-a26	77
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -BiFeO <sub>3</sub>	1C-a23	77
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -Bi <sub>4</sub> Ti <sub>5</sub> O <sub>12</sub>	1C-c9	84
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -CaTiO <sub>3</sub>	7B-6	114
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -Co <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	1C-a7	74
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -Co <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	1C-e11	87
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-e11	87
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -KNbO <sub>3</sub>	1C-d3	84
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -LaAlO <sub>3</sub>	1C-c5	83
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -Mn <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	1C-c8	83
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -Mn <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	1C-e11	87
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -NaNbO <sub>3</sub>	1C-e11	87
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -Ni <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	1C-c2	83
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -Ni <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	1C-e11	87
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-e11	87
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-b4	82
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a11	75
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-b3	82
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -CaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a9	75
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -CaTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f2	87
BaO <sub>5</sub> Ti	BaTiO <sub>3</sub> -CaTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f1	87

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Gross formula	Chemical formula	Nr.	Page
BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -LaInO <sub>3</sub> -LaYO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f12	88
BaO <sub>3</sub> Ti	BaTiO <sub>3</sub> -PbTiO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1C-f19	88
BaO <sub>3</sub> Ti	(Ba-Ca)(Ti-Zr)O <sub>3</sub>	1C-f15	88
BaO <sub>3</sub> Ti	(Ba-Pb)(Ti-Sn)O <sub>3</sub>	1C-f18	88
BaO <sub>3</sub> Ti	(Ba-Pb)(Ti-Zr)O <sub>3</sub>	1C-f17	88
BaO <sub>3</sub> U	BaUO <sub>3</sub> -BaTiO <sub>3</sub>	1C-a26	77
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub>	5C-j2	105
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -BaTiO <sub>3</sub>	1C-a23	77
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -CaZrO <sub>3</sub>	1C-a12	76
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -PbTiO <sub>3</sub>	1C-b9	82
BaO <sub>3</sub> Zr	BaZrO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a15	76
BaO <sub>3</sub> Zr	(Ba-Ca)(Zr-Ti)O <sub>3</sub>	1C-f15	88
BaO <sub>3</sub> Zr	(Ba-Pb)(Zr-Ti)O <sub>3</sub>	1C-f17	88
BaO <sub>3</sub> Zr	BaZr <sub>0.25</sub> Nb <sub>1.5</sub> O <sub>5.25</sub>	5C-j3	105
BeF <sub>4</sub> H <sub>8</sub> N <sub>2</sub>	(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub> -(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	14B-1	154
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -BaTiO <sub>3</sub>	1C-c9	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -LaAlO <sub>3</sub>	1C-b11	83
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -LaCrO <sub>3</sub>	1C-b12	83
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -LaFeO <sub>3</sub>	1C-a33	82
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1C-d23	85
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c13	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -PbZrO <sub>3</sub>	1C-c14	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -SrFeO <sub>3</sub>	1C-c16	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -Sr(Sn <sub>1/3</sub> Mn <sub>2/3</sub> )O <sub>3</sub>	1C-d22	85
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -SrSnO <sub>3</sub>	1C-c15	84
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -SrTiO <sub>3</sub>	1C-c7	83
BiFeO <sub>3</sub>	BiFeO <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f6	87
Bi <sub>5</sub> GaO <sub>15</sub> Ti <sub>3</sub>	Bi <sub>5</sub> Ti <sub>3</sub> GaO <sub>15</sub> -Bi <sub>4</sub> PbTi <sub>4</sub> O <sub>15</sub>	7B-7	114
BiSI	BiSI-SbSI	10B-5	128
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Ti	(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -BaTiO <sub>3</sub>	1C-d3	84
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Ti	(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-d20	85
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Ti	(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d5	84
Bi <sub>1/2</sub> K <sub>1/2</sub> O <sub>3</sub> Zr	(K <sub>1/2</sub> Bi <sub>1/2</sub> )ZrO <sub>3</sub> -PbZrO <sub>3</sub>	1C-d17	85
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-d20	85
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d4	84
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-d21	85
Bi <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Zr	(Na <sub>1/2</sub> Bi <sub>1/2</sub> )ZrO <sub>3</sub> -PbZrO <sub>3</sub>	1C-d16	85
BiNbO <sub>6</sub>	Bi(Nb-Ti)O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-14	102
Bi <sub>2</sub> Nb <sub>6</sub> O <sub>18</sub>	Bi <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-13	102
Bi <sub>2</sub> Nb <sub>6</sub> O <sub>18</sub>	Bi <sub>2</sub> PbNb <sub>2</sub> O <sub>9</sub> -Bi <sub>4</sub> TiNbO <sub>9</sub>	7B-1	113
Bi <sub>2</sub> Nb <sub>6</sub> O <sub>18</sub> Pb	Bi <sub>2</sub> PbNb <sub>2</sub> O <sub>9</sub> -BaBi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub>	7B-5	114
Bi <sub>2</sub> Nb <sub>6</sub> O <sub>18</sub> Pb	Bi <sub>2</sub> PbTi <sub>2</sub> NbO <sub>12</sub> -Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub>	7B-2	113
Bi <sub>3</sub> NbO <sub>12</sub> PbTi <sub>2</sub>	Bi <sub>2</sub> SrNb <sub>2</sub> O <sub>9</sub> -Bi <sub>3</sub> TiNbO <sub>9</sub>	7B-1	113
Bi <sub>2</sub> Nb <sub>2</sub> O <sub>9</sub> Sr	Bi <sub>3</sub> SrTi <sub>2</sub> NbO <sub>12</sub> -Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub>	7B-2	113
Bi <sub>3</sub> NbO <sub>12</sub> SrTi <sub>2</sub>	Bi <sub>4</sub> TiNbO <sub>9</sub> -Bi <sub>4</sub> BaNb <sub>2</sub> O <sub>9</sub>	7B-1	113
Bi <sub>3</sub> NbO <sub>9</sub> Ti	Bi <sub>3</sub> TiNbO <sub>9</sub> -Bi <sub>4</sub> PbNb <sub>2</sub> O <sub>9</sub>	7B-1	113
Bi <sub>3</sub> NbO <sub>9</sub> Ti	Bi <sub>3</sub> TiNbO <sub>9</sub> -Bi <sub>2</sub> SrNb <sub>2</sub> O <sub>9</sub>	7B-1	113
Bi <sub>3</sub> NbO <sub>9</sub> Ti	Bi <sub>4</sub> PbTi <sub>4</sub> O <sub>15</sub> -Bi <sub>5</sub> Ti <sub>3</sub> GaO <sub>15</sub>	7B-7	114
Bi <sub>4</sub> O <sub>15</sub> PbTi <sub>4</sub>	Bi <sub>4</sub> (Ti-Nb)O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-14	102
Bi <sub>4</sub> O <sub>15</sub> Ti	Bi <sub>4</sub> O <sub>3</sub> · 3TiO <sub>2</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-14	102
Bi <sub>2</sub> O <sub>9</sub> Ti <sub>3</sub>	Bi <sub>4</sub> O <sub>3</sub> · 3TiO <sub>2</sub> -SrTiO <sub>3</sub>	1C-e8	86
Bi <sub>2</sub> O <sub>9</sub> Ti <sub>3</sub>	Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> -BaTiO <sub>3</sub>	7B-6	114
Bi <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub>	Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> -Bi <sub>3</sub> BaTi <sub>2</sub> NbO <sub>12</sub>	7B-2	113
Bi <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub>	Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> -Bi <sub>3</sub> PbTi <sub>2</sub> NbO <sub>12</sub>	7B-2	113
Bi <sub>4</sub> O <sub>12</sub> Ti <sub>3</sub>	Bi <sub>4</sub> Ti <sub>3</sub> O <sub>12</sub> -Bi <sub>3</sub> SrTi <sub>2</sub> NbO <sub>12</sub>	7B-2	113
BrSSb	SbSBr-SbSI	10B-3	127
C <sub>6</sub> FH <sub>17</sub> N <sub>3</sub> O <sub>9</sub> P	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> PO <sub>3</sub> F-	28B-2	191
C <sub>6</sub> FeH <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SO <sub>4</sub>	22B-1	176
C <sub>6</sub> FeH <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-(NH <sub>4</sub> ) <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-2	176
C <sub>6</sub> FeH <sub>6</sub> K <sub>4</sub> N <sub>6</sub> O <sub>3</sub>	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-Rb <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-3	177
C <sub>6</sub> FeH <sub>16</sub> N <sub>10</sub> · 3H <sub>2</sub> O	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-Tl <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-1	176
C <sub>6</sub> FeH <sub>22</sub> N <sub>10</sub> O <sub>3</sub>	(NH <sub>4</sub> ) <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-1	176

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C <sub>6</sub> FeH <sub>5</sub> N <sub>6</sub> O <sub>9</sub> Rb <sub>4</sub>	Rb <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-2	176
C <sub>6</sub> FeH <sub>5</sub> N <sub>6</sub> O <sub>9</sub> Tl <sub>4</sub>	Tl <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-3	177
C <sub>6</sub> FeK <sub>4</sub> N <sub>6</sub> · 3H <sub>2</sub> O	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-(NH <sub>4</sub> ) <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-1	176
C <sub>6</sub> FeK <sub>4</sub> N <sub>6</sub> · 3H <sub>2</sub> O	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-Rb <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-2	176
C <sub>6</sub> FeK <sub>4</sub> N <sub>6</sub> · 3H <sub>2</sub> O	K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-Tl <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-3	177
C <sub>6</sub> FeN <sub>6</sub> Rb <sub>4</sub> · 3H <sub>2</sub> O	Rb <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-2	176
C <sub>6</sub> FeN <sub>6</sub> Tl <sub>4</sub> · 3H <sub>2</sub> O	Tl <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O-K <sub>4</sub> Fe(CN) <sub>6</sub> · 3H <sub>2</sub> O	22B-3	177
C <sub>4</sub> H <sub>4</sub> KNaO <sub>8</sub> · 4H <sub>2</sub> O	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O-NaNH <sub>4</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33B-1	198
C <sub>4</sub> H <sub>4</sub> KNaO <sub>8</sub> · 4H <sub>2</sub> O	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O-NaTlC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33B-2	198
C <sub>4</sub> H <sub>12</sub> KNaO <sub>10</sub>	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O-NaNH <sub>4</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33B-1	198
C <sub>4</sub> H <sub>12</sub> KNaO <sub>10</sub>	NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O-NaTlC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33B-2	198
C <sub>4</sub> H <sub>8</sub> NNaO <sub>6</sub> · 4H <sub>2</sub> O	NaNH <sub>4</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O-NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33B-1	198
C <sub>4</sub> H <sub>16</sub> NNaO <sub>10</sub>	NaNH <sub>4</sub> C <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O-NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33B-1	198
C <sub>6</sub> H <sub>17</sub> N <sub>3</sub> O <sub>10</sub> S	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SO <sub>4</sub> -(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> PO <sub>4</sub> F	28B-2	191
C <sub>6</sub> H <sub>17</sub> N <sub>3</sub> O <sub>10</sub> S	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SeO <sub>4</sub> -(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SeO <sub>4</sub>	28B-1	191
C <sub>6</sub> H <sub>17</sub> N <sub>3</sub> O <sub>10</sub> Se	(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SeO <sub>4</sub> -(NH <sub>2</sub> CH <sub>2</sub> COOH) <sub>3</sub> · H <sub>2</sub> SO <sub>4</sub>	28B-1	191
C <sub>4</sub> H <sub>4</sub> NaO <sub>6</sub> Tl · 4H <sub>2</sub> O	NaTlC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O-NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33B-2	198
C <sub>4</sub> H <sub>12</sub> NaO <sub>10</sub> Tl	NaTlC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O-NaKC <sub>4</sub> H <sub>4</sub> O <sub>6</sub> · 4H <sub>2</sub> O	33B-2	198
CaHfO <sub>3</sub>	CaHfO <sub>3</sub> -PbHfO <sub>3</sub>	1C-a16	76
CaNb <sub>2</sub> O <sub>6</sub>	CaNb <sub>2</sub> O <sub>6</sub> -BaNb <sub>2</sub> O <sub>6</sub>	5B-1	99
CaNb <sub>2</sub> O <sub>6</sub>	CaNb <sub>2</sub> O <sub>6</sub> -NaNb <sub>2</sub> O <sub>6</sub>	1C-e3	86
CaNb <sub>2</sub> O <sub>6</sub>	CaNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-2	99
CaNb <sub>2</sub> O <sub>6</sub>	(Ca-Ba-Pb)(Nb-Ta) <sub>2</sub> O <sub>6</sub>	5B-15	102
Ca <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Ca <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-1	106
CaO <sub>3</sub> Sn	CaSnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-b6	82
CaO <sub>3</sub> Sn	CaSnO <sub>3</sub> -SrSnO <sub>3</sub>	1C-a19	76
CaO <sub>3</sub> Sn	CaSnO <sub>3</sub> -SrSnO <sub>3</sub> -BaSnO <sub>3</sub>	1C-f13	88
CaO <sub>3</sub> Ta <sub>2</sub>	(Ca-Ba-Pb)(Ta-Nb) <sub>2</sub> O <sub>6</sub>	5B-15	102
Ca <sub>2</sub> O <sub>3</sub> Ta <sub>2</sub>	Ca <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -Sr <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	6B-6	106
CaO <sub>3</sub> Ti	CaTiO <sub>3</sub> -BaTiO <sub>3</sub>	1C-a7	74
CaO <sub>3</sub> Ti	CaTiO <sub>3</sub> -CaZrO <sub>3</sub>	1C-a22	76
CaO <sub>3</sub> Ti	CaTiO <sub>3</sub> -NaNbO <sub>3</sub>	1C-c1	83
CaO <sub>3</sub> Ti	CaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a8	75
CaO <sub>3</sub> Ti	CaTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-a6	74
CaO <sub>3</sub> Ti	CaTiO <sub>3</sub> -BaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f2	87
CaO <sub>3</sub> Ti	CaTiO <sub>3</sub> -BaTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f1	87
CaO <sub>3</sub> Ti	(Ca-Ba)(Ti-Zr)O <sub>3</sub>	1C-f15	88
CaO <sub>3</sub> Zr	CaZrO <sub>3</sub> -BaZrO <sub>3</sub>	1C-a12	76
CaO <sub>3</sub> Zr	CaZrO <sub>3</sub> -CaTiO <sub>3</sub>	1C-a22	76
CaO <sub>3</sub> Zr	CaZrO <sub>3</sub> -PbTiO <sub>3</sub>	1C-b5	82
CaO <sub>3</sub> Zr	CaZrO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a13	76
CaO <sub>3</sub> Zr	(Ca-Ba)(Zr-Ti)O <sub>3</sub>	1C-f15	88
CdNb <sub>2</sub> O <sub>6</sub>	CdNb <sub>2</sub> O <sub>6</sub> -NaNbO <sub>3</sub>	1C-e4	86
CdNb <sub>2</sub> O <sub>6</sub>	CdNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-10	101
Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Ca <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-1	106
Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Cd <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	6B-3	106
Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Mg <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-4	106
Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Pb <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-2	106
Cd <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	Cd <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-3	106
CdO <sub>3</sub> Ti	CdTiO <sub>3</sub> -LiNbO <sub>3</sub>	1C-e7	86
CdO <sub>3</sub> Ti	CdTiO <sub>3</sub> -LiTaO <sub>3</sub>	1C-e7	86
Ce <sub>1/3</sub> Li <sub>1/3</sub> O <sub>3</sub> Ti	(Li <sub>1/2</sub> Ce <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d8	85
CoLaO <sub>3</sub>	LaCoO <sub>3</sub> -PbTiO <sub>3</sub> -LaMnO <sub>3</sub>	1C-f11	87
Co <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Co <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	1C-e11	87
Co <sub>2</sub> O <sub>3</sub> Ta <sub>2</sub>	Co <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	1C-e11	87
CrLaO <sub>3</sub>	LaCrO <sub>3</sub> -BiFeO <sub>3</sub>	1C-b12	83
CrLaO <sub>3</sub>	LaCrO <sub>3</sub> -PbTiO <sub>3</sub> -LaMnO <sub>3</sub>	1C-f11	87
CsNO <sub>3</sub>	CsNO <sub>3</sub> -RbNO <sub>3</sub>	12B-4	134
Eu <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Eu-Gd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-5	201
Eu <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Eu-Tb) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-6	201

V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
FeLaO <sub>3</sub>	LaFeO <sub>3</sub> -BiFeO <sub>3</sub>	1C-a33	82
FeLaO <sub>3</sub>	LaFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c12	84
FeLaO <sub>3</sub>	LaFeO <sub>3</sub> -PbTiO <sub>3</sub> -LaMnO <sub>3</sub>	1C-f11	87
FeLaO <sub>3</sub>	LaFeO <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f5	87
Fe <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> )O <sub>3</sub> -BiFeO <sub>3</sub>	1C-d23	85
Fe <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> )O <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f8	87
Fe <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> -PbTiO <sub>3</sub>	1C-d11	85
Fe <sub>1/2</sub> O <sub>3</sub> PbTa <sub>1/2</sub>	Pb(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> -PbZrO <sub>3</sub>	1C-d15	85
FeO <sub>3</sub> Sr	SrFeO <sub>3</sub> -BiFeO <sub>3</sub>	1C-c16	84
Fe <sub>1/2</sub> O <sub>3</sub> SrTa <sub>1/2</sub>	Sr(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub> -SrTiO <sub>3</sub>	1C-d1	84
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Gd-Eu) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-5	201
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Gd-Nd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-8	202
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Gd-Tb) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-9	202
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	(Gd-Y) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-7	202
Gd <sub>2</sub> Mo <sub>3</sub> O <sub>12</sub>	Gd <sub>2</sub> ((Mo-W)O <sub>4</sub> ) <sub>3</sub>	35-10	202
Gd <sub>2</sub> O <sub>12</sub> W <sub>3</sub>	Gd <sub>2</sub> ((W-Mo)O <sub>4</sub> ) <sub>3</sub>	35-10	202
GeTe	GeTe-SnTe	36-3	214
H <sub>2</sub> KO <sub>4</sub> P	KH <sub>2</sub> PO <sub>4</sub> -NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	13B-1	148
H <sub>4</sub> N <sub>2</sub> O <sub>3</sub>	NH <sub>4</sub> NO <sub>3</sub> -KNO <sub>3</sub>	12B-1	134
H <sub>6</sub> NO <sub>4</sub> P	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> -KH <sub>2</sub> PO <sub>4</sub>	13B-1	148
H <sub>6</sub> NO <sub>4</sub> P	NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub> -TiH <sub>2</sub> PO <sub>4</sub>	13B-2	148
H <sub>8</sub> N <sub>2</sub> O <sub>4</sub> S	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> -(NH <sub>4</sub> ) <sub>2</sub> BeF <sub>4</sub>	14B-1	154
H <sub>2</sub> O <sub>4</sub> PTl	TiH <sub>2</sub> PO <sub>4</sub> -NH <sub>4</sub> H <sub>2</sub> PO <sub>4</sub>	13B-2	148
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -BaHfO <sub>3</sub>	1C-a18	76
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -CaHfO <sub>3</sub>	1C-a16	76
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -Pb(Sc <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1C-d18	85
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a29	82
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a31	82
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -SrHfO <sub>3</sub>	1C-a17	76
HfO <sub>3</sub> Pb	PbHfO <sub>3</sub> -PbTiO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-f4	87
HfO <sub>3</sub> Sr	SrHfO <sub>3</sub> -PbHfO <sub>3</sub>	1C-a17	76
IK	KI-KNO <sub>3</sub>	12B-3	134
IOSb	SbOI-SbSI	10B-2	127
ISSb	SbSI-AssI	10B-1	127
ISSb	SbSI-BiSI	10B-5	128
ISSb	SbSI-SbOI	10B-2	127
ISSb	SbSI-SbSBr	10B-3	127
ISSb	SbSI-SbSeI	10B-4	128
ISbSe	SbSeI-SbSI	10B-4	128
InLaO <sub>3</sub>	LaInO <sub>3</sub> -BaTiO <sub>3</sub> -LaYO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f12	88
KNO <sub>3</sub>	KNO <sub>3</sub> -KI	12B-3	134
KNO <sub>3</sub>	KNO <sub>3</sub> -NH <sub>4</sub> NO <sub>3</sub>	12B-1	134
KNO <sub>3</sub>	KNO <sub>3</sub> -RbNO <sub>3</sub>	12B-2	134
KNbO <sub>3</sub>	KNbO <sub>3</sub> -BaTiO <sub>3</sub>	1C-c5	83
KNbO <sub>3</sub>	KNbO <sub>3</sub> -KTaO <sub>3</sub>	1C-a4	74
KNbO <sub>3</sub>	KNbO <sub>3</sub> -NaNbO <sub>3</sub>	1C-a1	73
KNbO <sub>3</sub>	KNbO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-11	101
KNbO <sub>3</sub>	KNbO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c6	83
KNbO <sub>3</sub>	KNbO <sub>3</sub> -SrNb <sub>2</sub> O <sub>6</sub>	5C-b6	103
KNbO <sub>3</sub>	(K-Na)(Nb-Ta)O <sub>3</sub>	1C-f14	88
KNbO <sub>3</sub>	K <sub>0.6</sub> Li <sub>0.4</sub> (Nb <sub>0.3</sub> Ta <sub>0.7</sub> )O <sub>3</sub>	5C-k2	105
KNbO <sub>3</sub>	K(Nb <sub>0.65</sub> Ta <sub>0.35</sub> )O <sub>3</sub> (KTN)	1C-a5	74
KO <sub>3</sub> Sb	KSbO <sub>3</sub> -NaNbO <sub>3</sub>	1C-b2	82
KO <sub>3</sub> Ta	KTaO <sub>3</sub> -KNbO <sub>3</sub>	1C-a4	74
KO <sub>3</sub> Ta	KTaO <sub>3</sub> -NaNbO <sub>3</sub>	1C-b1	82
KO <sub>3</sub> Ta	K(Ta <sub>0.35</sub> Nb <sub>0.65</sub> )O <sub>3</sub> (KTN)	1C-a5	74
KO <sub>3</sub> Ta	(K-Na)(Ta <sub>0.7</sub> Nb <sub>0.3</sub> )O <sub>3</sub>	1C-f14	88
KO <sub>3</sub> Ta	K <sub>0.6</sub> Li <sub>0.4</sub> (Ta <sub>0.7</sub> Nb <sub>0.3</sub> )O <sub>3</sub>	5C-k2	105
KO <sub>3</sub> Ta	K(Ta <sub>0.35</sub> Nb <sub>0.65</sub> )O <sub>3</sub>	1C-a5	74
KTN			

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Page	Gross formula	Chemical formula	Nr.	Page
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84	La <sub>1/2</sub> Li <sub>1/2</sub> O <sub>3</sub> Ti	(Li <sub>1/2</sub> ,La <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d6	84
87	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-c11	84
87	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -LaCoO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
85	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -LaCrO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
87	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -LaFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
85	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -LaNiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
85	LaMnO <sub>3</sub>	LaMnO <sub>3</sub> -PbTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f10	87
84	La <sub>1/2</sub> Na <sub>1/2</sub> O <sub>3</sub> Ti	(Na <sub>1/2</sub> ,La <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d7	85
84	La <sub>2</sub> Nb <sub>6</sub> O <sub>18</sub>	La <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-12	101
201	LaNiO <sub>3</sub>	LaNiO <sub>3</sub> -LaMnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f11	87
202	La <sub>2</sub> O <sub>3</sub> Y	LaYO <sub>3</sub> -BaTiO <sub>3</sub> -LaInO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f12	88
202	LiNbO <sub>3</sub>	LiNbO <sub>3</sub> -CdTiO <sub>3</sub>	1C-e7	86
202	LiNbO <sub>3</sub>	LiNbO <sub>3</sub> -LiTaO <sub>3</sub>	3B-1	94
202	LiNbO <sub>3</sub>	LiNbO <sub>3</sub> -NaNbO <sub>3</sub>	1C-e1	86
202	LiNbO <sub>3</sub>	LiNbO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-11	101
214	Li <sub>1/2</sub> Nd <sub>1/2</sub> O <sub>3</sub> Ti	Li <sub>0.4</sub> K <sub>0.6</sub> (Nb <sub>0.3</sub> Ta <sub>0.7</sub> )O <sub>3</sub>	5C-k2	105
	LiO <sub>3</sub> Ta	(Li <sub>1/2</sub> ,Nd <sub>1/2</sub> )TiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-d9	85
148	LiO <sub>3</sub> Ta	LiTaO <sub>3</sub> -CdTiO <sub>3</sub>	1C-e7	86
134	LiO <sub>3</sub> Ta	LiTaO <sub>3</sub> -LiNbO <sub>3</sub>	3B-1	94
148		Li <sub>0.4</sub> K <sub>0.6</sub> (Ta <sub>0.7</sub> Nb <sub>0.3</sub> )O <sub>3</sub>	5C-k2	105
148	Mg <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Mg <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-4	106
154	Mg <sub>1/3</sub> Nb <sub>2/3</sub> O <sub>3</sub> Pb	Pb(Mg <sub>1/3</sub> ,Nb <sub>2/3</sub> )O <sub>3</sub> -Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1C-d19	85
148	Mg <sub>1/3</sub> Nb <sub>2/3</sub> O <sub>3</sub> Pb	Pb(Mg <sub>1/3</sub> ,Nb <sub>2/3</sub> )O <sub>3</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f7	87
76	Mg <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub> -Pb(Mg <sub>1/3</sub> ,Nb <sub>2/3</sub> )O <sub>3</sub>	1C-d19	85
76	Mg <sub>1/2</sub> O <sub>3</sub> PbW <sub>1/2</sub>	Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub> -PbTiO <sub>3</sub>	1C-d10	85
85	Mn <sub>1/2</sub> Nb <sub>1/2</sub> O <sub>3</sub> Pb	Pb(Mn <sub>1/2</sub> ,Nb <sub>1/2</sub> )O <sub>3</sub> -PbTiO <sub>3</sub>	1C-d13	85
82	Mn <sub>2/3</sub> O <sub>3</sub> Sn <sub>1/3</sub> Sr	Sr(Sn <sub>1/3</sub> ,Mn <sub>2/3</sub> )O <sub>3</sub> -BiFeO <sub>3</sub>	1C-d22	85
82	Mn <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	Mn <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	1C-e11	87
76	Mn <sub>2</sub> O <sub>3</sub> Ta <sub>2</sub>	Mn <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	1C-e11	87
87	Mo <sub>3</sub> Nd <sub>2</sub> O <sub>12</sub>	(Nd-Gd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-8	202
76	Mo <sub>3</sub> O <sub>12</sub> Tb <sub>2</sub>	(Tb-Eu) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-6	201
	Mo <sub>3</sub> O <sub>12</sub> Tb <sub>2</sub>	(Tb-Gd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-9	202
	Mo <sub>4</sub> O <sub>12</sub> Y <sub>2</sub>	(Y-Gd) <sub>2</sub> (MoO <sub>4</sub> ) <sub>3</sub>	35-7	202
134	NO <sub>3</sub> Rb	RbNO <sub>3</sub> -CsNO <sub>3</sub>	12B-4	134
127	NO <sub>3</sub> Rb	RbNO <sub>3</sub> -KNO <sub>3</sub>	12B-2	134
128	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -BaTiO <sub>3</sub>	1C-c2	83
127	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -CaNb <sub>2</sub> O <sub>6</sub>	1C-e3	86
128	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -CaTiO <sub>3</sub>	1C-c1	83
128	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -CdNb <sub>2</sub> O <sub>6</sub>	1C-e4	86
88	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -KNbO <sub>3</sub>	1C-a1	73
	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -KSbO <sub>3</sub>	1C-b2	82
134	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -KTaO <sub>3</sub>	1C-b1	82
134	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -LiNbO <sub>3</sub>	1C-e1	86
134	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -NaVO <sub>3</sub>	1C-e2	86
83	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -NaSbO <sub>3</sub>	1C-a3	74
74	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -NaTaO <sub>3</sub>	1C-a2	74
73	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1C-e6	86
101	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -PbTiO <sub>3</sub>	5B-11	101
83	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -PbZrO <sub>3</sub>	1C-c3	83
103	NaNbO <sub>3</sub>	NaNbO <sub>3</sub> -SrNb <sub>2</sub> O <sub>6</sub>	1C-c4	83
88	NaNbO <sub>3</sub>	(Na-K)(Nb-Ta)O <sub>3</sub>	1C-e5	86
105	NaO <sub>3</sub> Sb	NaSbO <sub>3</sub> -NaNbO <sub>3</sub>	1C-f14	88
74	NaO <sub>3</sub> Ta	NaTaO <sub>3</sub> -NaNbO <sub>3</sub>	1C-a3	74
82	NaO <sub>3</sub> Ta	(Na-K)(Ta-Nb)O <sub>3</sub>	1C-a2	74
74	NaO <sub>3</sub> V	NaVO <sub>3</sub> -NaNbO <sub>3</sub>	1C-f14	88
82	Nb <sub>2</sub> Ni <sub>2</sub> O <sub>7</sub>	Ni <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	1C-e2	86
74	Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -BaNb <sub>2</sub> O <sub>6</sub>	1C-e11	87
88	Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -Bi <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>6</sub>	5B-5	100
105	Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -Bi <sub>2</sub> O <sub>3</sub> · 3TiO <sub>2</sub>	5B-13	102
74	Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -CaNb <sub>2</sub> O <sub>6</sub>	5B-14	102
			5B-2	99

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Gross formula	Chemical formula	Nr.	Page
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -CdNb <sub>2</sub> O <sub>6</sub>	5B-10	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -KNbO <sub>3</sub>	5B-11	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -La <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub>	5B-12	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -LiNbO <sub>3</sub>	5B-11	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -NaNbO <sub>3</sub>	1C-e6,	86
Nb <sub>2</sub> O <sub>6</sub> Pb		5B-11	101
Nb <sub>2</sub> O <sub>6</sub> Pb		5B-9	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -PbO:SnO <sub>2</sub>	5B-6	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -PbTa <sub>2</sub> O <sub>6</sub>	5B-7	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -PbTiO <sub>3</sub>	5B-8,	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -PbZrO <sub>3</sub>	1C-e12	87
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -RbNbO <sub>3</sub>	5B-11	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -Sm <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub>	5B-12	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -SrNb <sub>2</sub> O <sub>6</sub>	5B-4	100
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -Y <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub>	5B-12	101
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -Bi(Nb-Ti)O <sub>6</sub>	5B-14	102
Nb <sub>2</sub> O <sub>6</sub> Pb	PbNb <sub>2</sub> O <sub>6</sub> -BaNb <sub>2</sub> O <sub>6</sub> -BaTiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f19	88
Nb <sub>2</sub> O <sub>6</sub> Pb	(Pb-Ba-Ca)(Nb-Ta) <sub>2</sub> O <sub>6</sub>	5B-15	102
Nb <sub>2</sub> O <sub>6</sub> Pb	(Pb-Ba-Sr)(Nb-Ta) <sub>2</sub> O <sub>6</sub>	5B-15	102
Nb <sub>2</sub> O <sub>6</sub> Pb	Pb <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Cd <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-2	106
Nb <sub>2</sub> O <sub>6</sub> Pb <sub>2</sub>	Pb <sub>2</sub> (Sc <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>7</sub> -PbHfO <sub>3</sub>	1C-d18	85
Nb <sub>1/2</sub> O <sub>3</sub> PbSc <sub>1/2</sub>	Pb <sub>2</sub> (Sc <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>7</sub> -PbTiO <sub>3</sub>	1C-d12	85
Nb <sub>1/2</sub> O <sub>3</sub> PbSc <sub>1/2</sub>	Pb <sub>2</sub> (Sc <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>7</sub> -PbZrO <sub>3</sub>	1C-d14	85
Nb <sub>1/2</sub> O <sub>3</sub> PbSc <sub>1/2</sub>	RbNbO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-11	101
Nb <sub>3</sub> O <sub>5</sub> Rb	Sm <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-12	101
Nb <sub>6</sub> O <sub>18</sub> Sm <sub>2</sub>	Sm <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-3	99
Nb <sub>2</sub> O <sub>6</sub> Sr	SrNb <sub>2</sub> O <sub>6</sub> -BaNb <sub>2</sub> O <sub>6</sub>	5C-b6	103
Nb <sub>2</sub> O <sub>6</sub> Sr	SrNb <sub>2</sub> O <sub>6</sub> -KNbO <sub>3</sub>	1C-e5	86
Nb <sub>2</sub> O <sub>6</sub> Sr	SrNb <sub>2</sub> O <sub>6</sub> -NaNbO <sub>3</sub>	5B-4	100
Nb <sub>2</sub> O <sub>6</sub> Sr	SrNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-15	102
Nb <sub>2</sub> O <sub>6</sub> Sr	(Sr-Ba-Pb)(Nb-Ta) <sub>2</sub> O <sub>6</sub>	6B-5	106
Nb <sub>2</sub> O <sub>6</sub> Sr	Sr <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub> -Sr <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	1C-e11	87
Nb <sub>2</sub> O <sub>7</sub> Sr <sub>2</sub>	Ni <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -BaTiO <sub>3</sub>	5B-12	101
Ni <sub>2</sub> O <sub>7</sub> Ta <sub>2</sub>	Y <sub>2</sub> O <sub>3</sub> · 3Nb <sub>2</sub> O <sub>5</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1C-a21	76
Nb <sub>2</sub> O <sub>18</sub> Y <sub>2</sub>	PbO:SnO <sub>2</sub> -BaSnO <sub>3</sub>	1C-b4	82
O <sub>3</sub> PbSn	PbO:SnO <sub>2</sub> -BaTiO <sub>3</sub>	5B-9	101
O <sub>3</sub> PbSn	PbO:SnO <sub>2</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1C-a30	82
O <sub>3</sub> PbSn	PbO:SnO <sub>2</sub> -PbTiO <sub>3</sub>	1C-a32	82
O <sub>3</sub> PbSn	PbO:SnO <sub>2</sub> -PbZrO <sub>3</sub>	1C-f4	87
O <sub>3</sub> PbSn	PbO:SnO <sub>2</sub> -PbHfO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f3	87
O <sub>3</sub> PbSn	PbO:SnO <sub>2</sub> -PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f18	88
O <sub>3</sub> PbSn	(Pb-Ba)(Sn-Ti)O <sub>3</sub>	5B-6	101
O <sub>6</sub> PbTa <sub>2</sub>	PbTa <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1C-e13	87
O <sub>6</sub> PbTa <sub>2</sub>	PbTa <sub>2</sub> O <sub>6</sub> -PbZrO <sub>3</sub>	5B-16	102
O <sub>6</sub> PbTa <sub>2</sub>	PbTa <sub>2</sub> O <sub>6</sub> -SrTa <sub>2</sub> O <sub>6</sub>	5B-15	102
O <sub>6</sub> PbTa <sub>2</sub>	(Pb-Ba-Ca)(Ta-Nb) <sub>2</sub> O <sub>6</sub>	5B-15	102
O <sub>6</sub> PbTa <sub>2</sub>	(Pb-Ba-Sr)(Ta-Nb) <sub>2</sub> O <sub>6</sub>	1C-b10	83
O <sub>6</sub> PbTa <sub>2</sub>	PbTiO <sub>3</sub> -BaSnO <sub>3</sub>	1C-a11	75
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -BaTiO <sub>3</sub>	1C-b9	82
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -BaZrO <sub>3</sub>	1C-c13	84
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -BiFeO <sub>3</sub>	1C-b6	82
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -CaSnO <sub>3</sub>	1C-a8	75
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -CaTiO <sub>3</sub>	1C-b5	82
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -CaZrO <sub>3</sub>	1C-d5	84
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -(K <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-c6	83
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -KNbO <sub>3</sub>	1C-c10	84
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaAlO <sub>3</sub>	1C-c12	84
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaFeO <sub>3</sub>	1C-c11	84
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaMnO <sub>3</sub>	1C-d8	85
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -(Li <sub>1/2</sub> Ce <sub>1/2</sub> )TiO <sub>3</sub>	1C-d6	84
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -(Li <sub>1/2</sub> La <sub>1/2</sub> )TiO <sub>3</sub>	1C-d9	85
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -(Li <sub>1/2</sub> Nd <sub>1/2</sub> )TiO <sub>3</sub>	1C-d4	84
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-d7	85
O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -(Na <sub>1/2</sub> La <sub>1/2</sub> )TiO <sub>3</sub>		

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Page	Gross formula	Chemical formula	Nr.	Page
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -NaNbO <sub>3</sub>	1C-c3	83
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -Pb(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1C-d11	85
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -PbHfO <sub>3</sub>	1C-a29	82
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -Pb(Mg <sub>1/2</sub> W <sub>1/2</sub> )O <sub>3</sub>	1C-d10	85
86	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -Pb(Mn <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1C-d13	85
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-7	101
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-a30	82
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -Pb(Sc <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub>	1C-d12	85
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a27	77
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -SrSnO <sub>3</sub>	1C-b8	82
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -SrTiO <sub>3</sub>	1C-a10	75
87	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -SrZrO <sub>3</sub>	1C-b7	82
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -ABO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f9	87
100	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -BaTiO <sub>3</sub> -CaTiO <sub>3</sub>	1C-f2	87
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -BiFeO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f6	87
102	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaCoO <sub>3</sub> -LaMnO <sub>3</sub>	1C-f11	87
88	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaCrO <sub>3</sub> -LaMnO <sub>3</sub>	1C-f11	87
102	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaFeO <sub>3</sub> -LaMnO <sub>3</sub>	1C-f11	87
102	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaFeO <sub>3</sub> -PbZrO <sub>3</sub>	1C-f5	87
106	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaMnO <sub>3</sub> -LaNiO <sub>3</sub>	1C-f11	87
85	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -LaMnO <sub>3</sub> -SrTiO <sub>3</sub>	1C-f10	87
85	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub> -PbZrO <sub>3</sub>	1C-f8	87
85	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -PbHfO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-f4	87
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub> -PbZrO <sub>3</sub>	1C-f7	87
101	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -PbO:SnO <sub>2</sub> -PbZrO <sub>3</sub>	1C-f3	87
99	O <sub>3</sub> PbTi	PbTiO <sub>3</sub> -BaTiO <sub>3</sub> -BaNb <sub>2</sub> O <sub>6</sub> -PbNb <sub>2</sub> O <sub>6</sub>	1C-f19	88
103	O <sub>3</sub> PbTi	(Pb-Ba)(Ti-Sn)O <sub>3</sub>	1C-f18	88
86	O <sub>3</sub> PbTi	(Pb-Ba)(Ti-Zr)O <sub>3</sub>	1C-f17	88
100	O <sub>3</sub> PbTi	Pb(Ti-Zr)O <sub>3</sub>	1C-a28	78
102	O <sub>3</sub> PbTi	(Pb-Sr)(Ti-Zr)O <sub>3</sub>	1C-f16	88
106	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -BaTiO <sub>3</sub>	1C-b3	82
87	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -BaZrO <sub>3</sub>	1C-a15	76
101	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -BiFeO <sub>3</sub>	1C-c14	84
76	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -CaZrO <sub>3</sub>	1C-a13	76
82	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -(K <sub>1/2</sub> Bi <sub>1/2</sub> )ZrO <sub>3</sub>	1C-d17	85
101	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -(Na <sub>1/2</sub> Bi <sub>1/2</sub> )TiO <sub>3</sub>	1C-d21	85
82	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -(Na <sub>1/2</sub> Bi <sub>1/2</sub> )ZrO <sub>3</sub>	1C-d16	85
82	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -NaNbO <sub>3</sub>	1C-c4	83
87	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -Pb(Fe <sub>1/2</sub> Ta <sub>1/2</sub> )O <sub>3</sub>	1C-d15	85
87	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -PbHfO <sub>3</sub>	1C-a31	82
87	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -PbNb <sub>2</sub> O <sub>6</sub>	5B-8,	101
88	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -PbO:SnO <sub>2</sub>	1C-e12	87
101	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -Pb(Sc <sub>1/4</sub> Nb <sub>1/4</sub> )O <sub>3</sub>	1C-a32	82
87	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -PbTa <sub>2</sub> O <sub>6</sub>	1C-d14	85
102	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -PbTiO <sub>3</sub>	1C-e13	87
102	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -SrZrO <sub>3</sub>	1C-a27	77
83	O <sub>3</sub> PbZr	Pb(Zr-Ti)O <sub>3</sub> (PZT)	1C-a14	76
75	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -ABO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a28	78
82	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -BiFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f9	87
84	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -LaFeO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f6	87
82	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -Pb(Fe <sub>1/2</sub> Nb <sub>1/2</sub> )O <sub>3</sub> -PbTiO <sub>3</sub>	1C-f5	87
75	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -Pb(Mg <sub>1/3</sub> Nb <sub>2/3</sub> )O <sub>3</sub> -PbTiO <sub>3</sub>	1C-f8	87
82	O <sub>3</sub> PbZr	PbZrO <sub>3</sub> -PbO:SnO <sub>2</sub> -PbTiO <sub>3</sub>	1C-f7	87
84	O <sub>3</sub> PbZr	(Pb-Ba)(Zr-Ti)O <sub>3</sub>	1C-f3	87
83	O <sub>3</sub> PbZr	(Pb-Sr)(Zr-Ti)O <sub>3</sub>	1C-f17	88
84	O <sub>3</sub> SnSr	SrSnO <sub>3</sub> -BaSnO <sub>3</sub>	1C-f16	88
84	O <sub>3</sub> SnSr	SrSnO <sub>3</sub> -BiFeO <sub>3</sub>	1C-a20	76
84	O <sub>3</sub> SnSr	SrSnO <sub>3</sub> -CaSnO <sub>3</sub>	1C-c15	84
85	O <sub>3</sub> SnSr	SrSnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a19	76
84	O <sub>6</sub> SrTa <sub>2</sub>	SrSnO <sub>3</sub> -BaSnO <sub>3</sub> -CaSnO <sub>3</sub>	1C-b8	82
85	O <sub>6</sub> SrTa <sub>2</sub>	SrTa <sub>2</sub> O <sub>6</sub> -PbTa <sub>2</sub> O <sub>6</sub>	1C-f13	88
84	O <sub>7</sub> Sr <sub>2</sub> Ta <sub>2</sub>	(Sr-Ba-Pb)(Ta-Nb) <sub>2</sub> O <sub>6</sub>	5B-16	102
85	O <sub>7</sub> Sr <sub>2</sub> Ta <sub>2</sub>	Sr <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -Ca <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	5B-15	102
85	O <sub>7</sub> Sr <sub>2</sub> Ta <sub>2</sub>	Sr <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -Ca <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub>	6B-6	106

V Substanzenverzeichnis

Gross formula	Chemical formula	Nr.	Page
O <sub>2</sub> Sr <sub>2</sub> Ta <sub>2</sub>	Sr <sub>2</sub> Ta <sub>2</sub> O <sub>7</sub> -Sr <sub>2</sub> Nb <sub>2</sub> O <sub>7</sub>	6B-5	106
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -BaTiO <sub>3</sub>	1C-a9	75
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -BiFeO <sub>3</sub>	1C-c7	83
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -B <sub>2</sub> O <sub>3</sub> · 3TiO <sub>2</sub>	1C-e8	86
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -CaTiO <sub>3</sub>	1C-a6	74
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -PbTiO <sub>3</sub>	1C-a10	75
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -Sr(Fe <sub>1/3</sub> Ta <sub>1/3</sub> )O <sub>2</sub>	1C-d1	84
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -BaTiO <sub>3</sub> -CaTiO <sub>3</sub>	1C-f1	87
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -LaMnO <sub>3</sub> -PbTiO <sub>3</sub>	1C-f10	87
O <sub>2</sub> SrTi	SrTiO <sub>3</sub> -BaTiO <sub>3</sub> -LaInO <sub>3</sub> -LaYO <sub>3</sub>	1C-f12	88
O <sub>2</sub> SrZr	(Sr-Pb)(Ti-Zr)O <sub>3</sub>	1C-f16	88
O <sub>2</sub> SrZr	SrZrO <sub>3</sub> -PbTiO <sub>3</sub>	1C-b7	82
O <sub>2</sub> SrZr	SrZrO <sub>3</sub> -PbZrO <sub>3</sub>	1C-a14	76
O <sub>2</sub> SrZr	(Sr-Pb)(Zr-Ti)O <sub>3</sub>	1C-f16	88
PZT	Pb(Zr-Ti)O <sub>3</sub>	1C-a28	78
SnTe	SnTe-GeTe	36-3	214

# **BRIEF ATTACHMENT Q**

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**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT Q**

J. G. Becker

STRUCTURE AND  
PROPERTIES OF  
INORGANIC SOLIDS

BY

FRANCIS S. GALASSO

United Aircraft Research Laboratories

ILLUSTRATED BY

W. DARBY



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cell is elongated in the  $c$  direction; the lead atoms are displaced vertically downwards in the front and back faces and upwards in the side faces. This arrangement corresponds to placement of the atoms in the following special positions in space group  $P4/nmm$ :

$$\begin{aligned} \text{2Pb at } (2c) : 0, \frac{1}{4}, z; \frac{1}{2}, 0, \bar{z} \text{ with } z = 0.2385; \\ \text{2O at } (2a) : 0, 0, 0; \frac{1}{2}, \frac{1}{2}, 0. \end{aligned}$$

In this structure both the lead and oxygen atoms are in fourfold coordination with atoms of the other type. The oxygen atoms are in a tetrahedron of lead atoms, while the lead atoms are at the vertex of a square pyramid with oxygen atoms at the base. In the horizontal oxygen sheets, the atoms are in square planar coordination or roughly cubic packing. This structure is illustrated in Fig. 7.1. Other compounds which adopt this structure are listed in Table 7.1.

## CHAPTER 7 PEROVSKITE TYPE AND RELATED STRUCTURES

THE perovskite-type structures are formed by  $\text{ABX}_3$ -type compounds where the A atoms replace some of the X atoms in close-packed cubic layers and the B atoms fit in the octahedrally coordinated sites. In the ordered  $\text{Cu}_3\text{Au}$  structure there are no B atoms; in the  $\text{ReO}_3$  structure the A atoms are missing so that there are holes in the close-packed X atom layers. These close-packed layers are perpendicular to the  $\langle 111 \rangle$  directions (body diagonals) in the cubic unit cell. Related structures can be built up as close-packed layers of X atoms or by stacking cubic unit cells. The flow diagram showing the relationships between these structures is presented in Table 7.0.

TABLE 7.0.

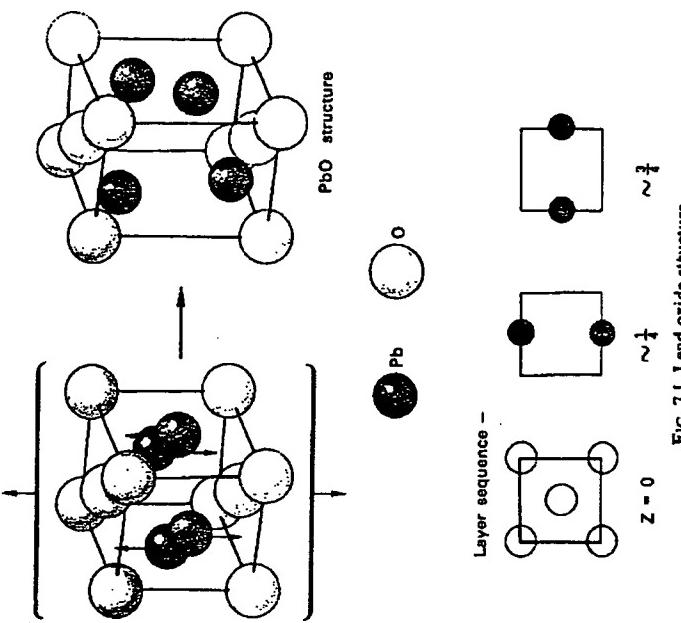
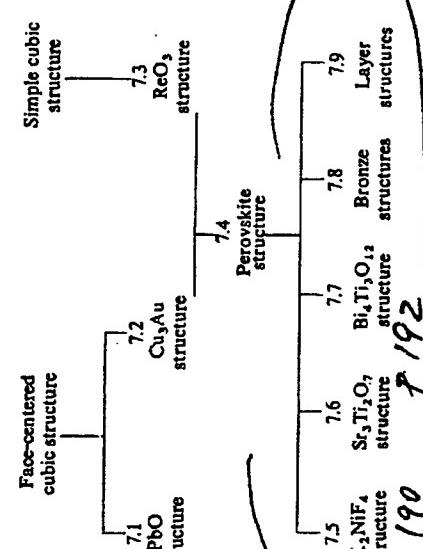


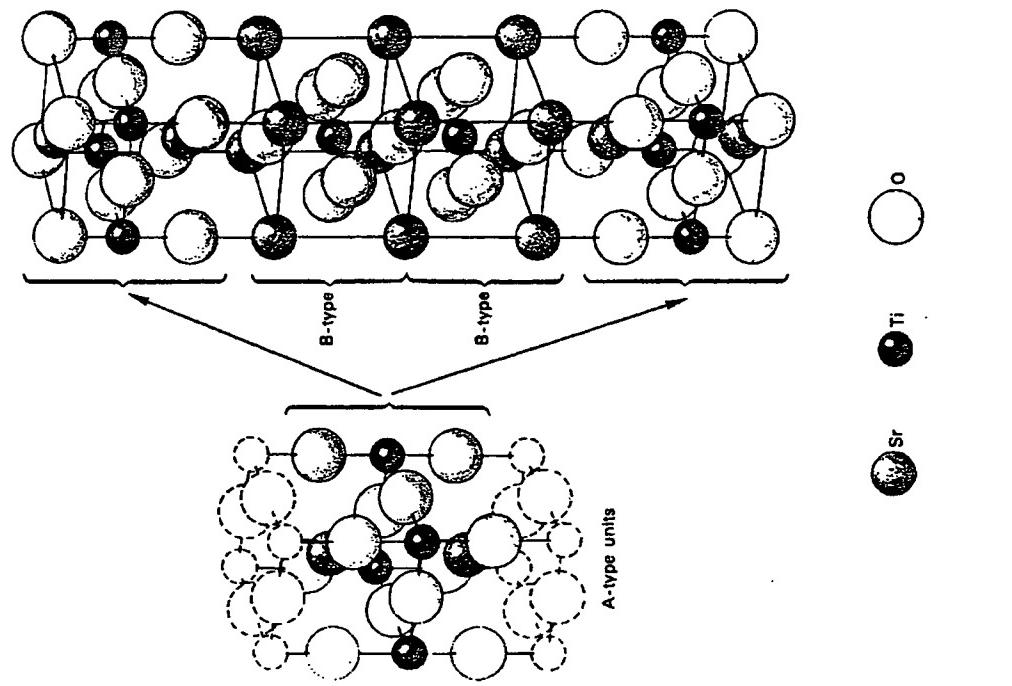
Fig. 7.1. Lead oxide structure

### 7.1. Red Lead Oxide, $\text{PbO}$ , $\text{BiO}$ , $\text{P}4/\text{pmm}$ , Tetragonal

This lead oxide structure can be visualized by starting with an ordered cubic close-packed structure. Lead atoms are placed in the centered positions on the vertical faces of a unit cell and the oxygen atoms in the centered position on the top and bottom faces as well as at the cell corners. The cubic

TABLE 7.5. Phases with the  $K_2NiF_4$  Structure

Phases	Cell size (Å)		Atomic parameters		Refs.
	$a_0$	$c_0$	$z(A \text{ cation})$	$z(\text{anion})$	
Halides, Oxyhalides					
$C_3CCl_4$	5.215	16.46			1
$K_2CoF_4$	4.074	13.08			2
$K_2CuF_4$	4.155	12.74	0.336	0.153	3
$K_2MgF_4$	3.977	13.16	0.35	0.15	4
$K_2NiF_4$	4.01	13.08	0.352	0.151	5
$K_2NbO_3F$	3.96	13.67			6
$K_2ZnF_4$	4.017	13.05			7
$(NH_4)_2NiF_4$	4.084	13.79			8
$Rb_2NiF_4$	4.087	13.71			8
$Rb_2ZnF_4$	4.104	13.28			7
$Sr_2FeO_3F$	3.84	12.98			9
$Tl_2CoF_4$	4.10	14.1			2
$Tl_2NiF_4$	4.051	14.22			8
Oxides					
$Ba_2PbO_4$	4.296	13.30	0.335	0.155	10
$Ba_2SnO_4$	4.130	13.27	0.335	0.155	10
$Ca_2MnO_4$	3.67	12.08			11
$Cs_2UO_4$	4.38	14.79			12
$Gd_2CuO_4$	3.89	11.85			13
$K_2UO_4$	4.34	13.10	0.36	0.145	14
$La_2NiO_4$	3.855	12.652	0.360	0.170	15
$Nd_2CuO_4$	3.94	12.15			13
$Nd_2NiO_4$	3.81	12.31			13
$Rb_2UO_4$	4.345	13.83			12
$Sm_2CuO_4$	3.91	11.93			13
$Si_2IrO_4$	3.89	12.92	0.347	0.151	16
$Si_2MnO_4$	3.79	12.43			5
$Si_2MoO_4$	3.92	12.84			5
$Si_2RhO_4$	3.85	12.90			17
$Si_2RuO_4$	3.870	12.74			17
$Si_2SnO_4$	4.037	12.53	0.353	0.153	19
$Si_2TiO_4$	3.884	12.60	0.353	0.152	18
Complex Oxides					
$La_2(Li_{0.5}Co_{0.5})O_4$	3.77	12.58			19
$La_2(Li_{0.5}Ni_{0.5})O_4$	3.75	12.89			19
$SrLaAlO_4$	3.75	12.5			11
$SrLaCoO_4$	3.80	12.50			19
$(Sr_{1-x}La_{x})_2(Co_{0.5}Ti_{0.5})O_4$	3.85	12.62			19
$SrLaCrO_4$	3.84	12.52			19
$(Sr_{0.5}La_{0.5})(Mg_{0.5}Co_{0.5})O_4$	3.82	12.58			19
$SrLaFeO_4$	3.86	12.69			19
$SrLaGaO_4$	3.84	12.71			19
$SrLaMnO_4$	3.88	12.5			19
$SrLaNiO_4$	3.80	12.51			19
$SrLaRhO_4$	3.92	12.78			19

FIG. 7.6 The  $Sr_3Ti_2O_7$  structure

The structure of  $\text{Sr}_4\text{Ti}_3\text{O}_{10}$  is similar but requires a longer  $c$ -axis to describe it. The cell sizes are listed in Table 7.6.

TABLE 7.6. Series of Sr-Ti-O Compounds

Compound	Cell size ( $\text{\AA}$ )	$a_0$	$c_0$	Refs.
$\text{Sr}_2\text{TiO}_4$	3.884	12.60	1	
$\text{Sr}_3\text{Ti}_2\text{O}_7$	3.90	20.38	2	
$\text{Sr}_4\text{Ti}_3\text{O}_{10}$	3.90	28.1	2	
$\text{K}_3\text{Zn}_2\text{F}_7$	4.063	21.22	3	

### 7.7. $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ Structure, $Fmmmm$ , Orthorhombic

$\text{Bi}_4\text{Ti}_3\text{O}_{12}$  is one of a series of ferroelectric compounds which can be best described by unit cells of the perovskite structure stacked on one another and separated by bismuth oxygen layers. The structures of  $\text{Bi}_2\text{NbO}_5\text{F}$ ,  $\text{Bi}_3\text{NbTiO}_9$  and  $\text{BaBi}_4\text{TiO}_{15}$  have been characterized, but in this book, only one,  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ , will be described. Half the unit cell consists of one and one-half A type perovskite unit cells with an oxygen layer on top and one and one-half B type perovskite unit cells on top of the oxygen layer. The top half of the cell is the mirror image of this one. The unit cell just described is shown in Fig. 7.7a inside the real cell. The actual  $a$  and  $b$  edges are taken as the face diagonals of the small unit cell of the perovskite structure. The layer sequence is shown in Fig. 7.7b. The atomic positions are given below:

		$x$	$y$	$z$
Bi(1)	(8i)	0	0	0.067
(2)	(8i)	0	0	0.211
Ti(1)	(4b)	0	0	0.50
(2)	(8i)	0	0	0.372
O(1)	(8e)	0.25	0.25	0
(2)	(8i)	0.25	0.25	0.25
(3)	(8i)	0	0	0.436
(4)	(8i)	0	0	0.308
(5)	(16j)	0.25	0.25	0.128
				(8)
(4b)	0, 0, $\frac{1}{2}; \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, 0, 0; 0, \frac{1}{2}, 0$			
(8e)	$\frac{1}{4}, \frac{1}{4}, 0; \frac{1}{4}, \frac{1}{4}, \frac{1}{2}$			
	$\frac{3}{4}, \frac{3}{4}, 0; \frac{3}{4}, \frac{3}{4}, \frac{1}{2}$			
	$\frac{3}{4}, \frac{1}{4}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 0$			
	$\frac{1}{4}, \frac{3}{4}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, 0$			

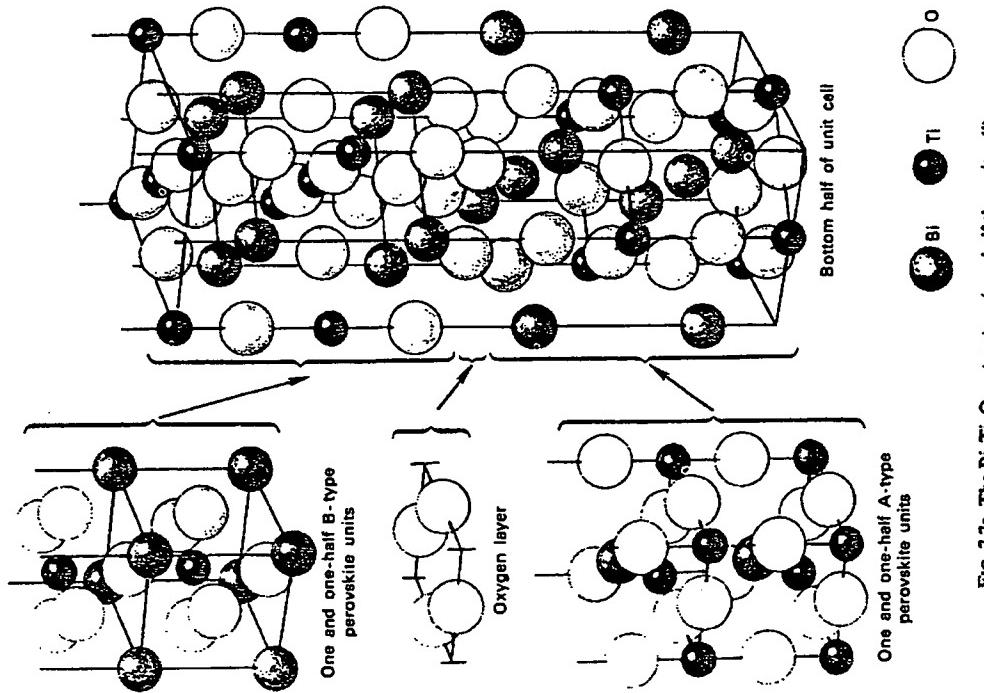


Fig. 7.7a. The  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  structure (one-half the unit cell).

### PERO SKITE TYPE AND RELATED STRUCTURES

- (8i)  $0, 0, z; \frac{1}{2}, \frac{1}{2}, z; \frac{1}{2}, 0, \frac{1}{2} + z; 0, \frac{1}{2} + z$
- 0, 0,  $z; \frac{1}{2}, \frac{1}{2}, 0, \frac{1}{2} - z; 0, \frac{1}{2} - z$
- (16j)  $\frac{1}{4}, \frac{1}{4}, z; \frac{1}{4}, \frac{1}{4}, \frac{1}{2}; \frac{1}{4}, \frac{1}{4}, \frac{3}{2}, \bar{z}$
- $\frac{3}{4}, \frac{3}{4}, z; \frac{3}{4}, \frac{3}{4}, \frac{1}{2}; \frac{3}{4}, \frac{3}{4}, \frac{1}{2}, \bar{z}$
- $\frac{3}{4}, \frac{1}{4}, \frac{1}{2} + z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2} + z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z$
- $\frac{1}{4}, \frac{3}{4}, \frac{1}{2} + z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2} - z; \frac{1}{2}, \frac{1}{2}, \frac{1}{2} + z$

**BRIEF ATTACHMENT R**

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P.O. Box 1450  
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**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT R**

# CRYSTAL STRUCTURES

Second Edition

Ralph W. G. Wyckoff, *University of Arizona, Tucson, Arizona*

## VOLUME 4

Miscellaneous Inorganic Compounds, Silicates, and  
Basic Structural Information

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## Preface

The presentation of data in this volume follows without significant change the pattern established in preceding volumes of this edition. As in Volume V, which was issued earlier, right-hand axes are used in all new drawings.

Since this edition was planned, it has been decided not to enlarge its scope by including intermetallic compounds. Instead, Chapter XIII is devoted to a very abbreviated statement of basic ideas about symmetry and valence. The writer has found that there are many people wishing to use structural data whose training has not prepared them to read with understanding the descriptions of structure now standard. Chapter XIII aims to give this information in as condensed a form as possible. Considering the rapidity with which valence theory is developing, its discussion of valence will undoubtedly seem inadequate to chemists concerned with the subject. In the writer's experience, however, there is little middle ground between a cursory statement such as that given here and a treatment, dealing mostly with organic structures, too long and detailed to be appropriate to the present series.

RALPH W. G. WYCKOFF

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TABLE XI,45  
Positions and Parameters of the Atoms in  $PbBi_2Nb_2O_9$

Atom	Position	$x$	$y$	$z$
Pb	(4a)	0	0	0.500
Bi	(8c)	0	0.50	0.200
Nb	(8c)	0	0.50	0.422
O(1)	(4a)	0	0	0.00
O(2)	(8b)	$\frac{1}{4}$	$\frac{1}{4}$	0.25
O(3)	(8b)	$\frac{1}{4}$	$\frac{1}{4}$	0.079
O(4)	(8b)	$\frac{1}{4}$	$\frac{1}{4}$	-0.079
O(5)	(8c)	0	0.50	0.158

with the parameters of Table XI,45.

This structure, like those of  $Bi_2Ti_3O_{10}$  (XI,512) and  $BaBi_4Ti_4O_{18}$  (XI,13) is built up of alternating  $Bi_2O_3$  and perovskite-like layers.

The following compounds are isostuctural:

Crystal	$a_0$ , Å.	$b_0$ , Å.	$c_0$ , Å.
$Bi_2Nb_2O_9$	5.533	5.533	25.55
$Bi_2Ta_2O_9$	5.402	6.436	25.15
$Bi_2TiNb_2O_9$	5.409	5.453	25.16
$CaBi_2Nb_2O_9$	5.425	5.485	24.87
$CaBi_2Ta_2O_9$	5.485	5.468	24.97
$SrBi_2Nb_2O_9$	5.504	5.504	26.06
$SrBi_2Ta_2O_9$	5.509	5.509	25.06
$KBi_2(Nb_2O_5)_2^*$	5.508	5.508	25.26
$NaBi_2(Nb_2O_5)_2^*$	5.47	5.47	26.94

\*Two molecules per cell.

At elevated temperatures  $a_0$  approaches  $b_0$  and the symmetry of these compounds becomes tetragonal.

XI,78. The oxychloride mineral *perite*,  $PbBi_2O_3Cl$ , is orthorhombic with a tetramolecular unit of the edge lengths:

$$a_0 = 5.627(50) \text{ Å}; b_0 = 5.575(20) \text{ Å}; c_0 = 12.425(90) \text{ Å}.$$

Its space group is  $V_h^{17}$  (*Bmm*) with atoms in the positions:

- Pb: (4c)  $\pm(0 \frac{1}{4} u; \frac{1}{2}, u + \frac{1}{2})$  with  $u = 0.385$
- Bi: (4c) with  $u = 0.090$
- Cl: (4c) with  $u = 0.75$
- O: (8e)  $\pm(u00; u \frac{1}{2} 0; u + \frac{1}{2}, 0 \frac{1}{2}; u + \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  with  $u = 0.25$

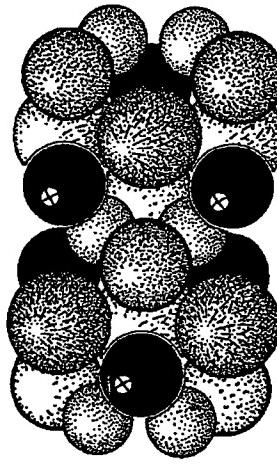
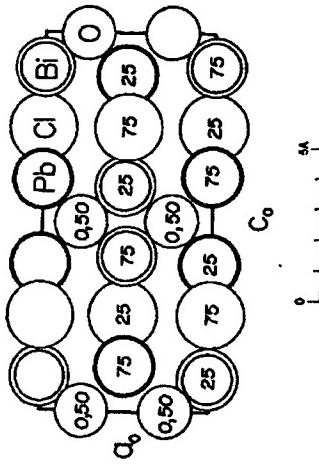


Fig. XI,60a (top). The orthorhombic structure of  $PbBi_2O_3Cl$  projected along its  $b$ -axis.

Fig. XI,60b (bottom). A packing drawing of the orthorhombic  $PbBi_2O_3Cl$  structure seen along its  $b$ -axis. The lead atoms are black; the bismuth are heavily outlined and black shaded. The still larger dot-and-line shaded circles are chlorine; atoms of oxygen are smaller and dotted.

The resulting structure is shown in Figure XI,60. Each lead atom has four oxygen neighbors 2.45 Å. away and four more distant chlorine atoms (3.25 and 3.30 Å.). The environment of bismuth is similar, with  $Bi-4O = 2.27$  Å. and  $Bi-4Cl = 3.42$  and 3.45 Å.

The corresponding antimony compound, which occurs as the mineral *Madorite*,  $PbSb_2O_3Cl$ , is isostructural. For it:

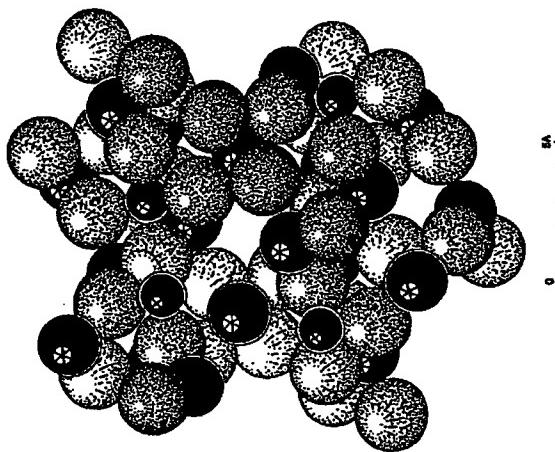
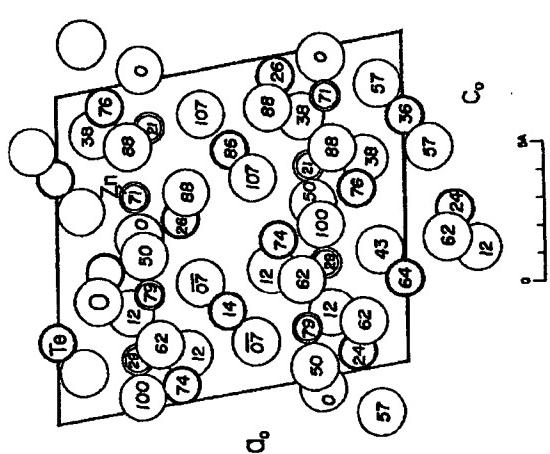
$$a_0 = 5.59 \text{ Å}; b_0 = 5.43 \text{ Å}; c_0 = 12.20 \text{ Å}.$$

The atomic positions and parameters are:

- Pb: (4c) with  $u = 0.380$
- Sb: (4c) with  $u = 0.078$
- Cl: (4c) with  $u = 0.756$
- O: (8e) with  $u = 0.25$

BIBLIOGRAPHY TABLE, CHAPTER XI

Compound	Paragraph	Literature
$\text{Ag}(\text{CN})_2$	2	1966; K&B
$\text{AgCN} \cdot 2\text{AgNO}_3$	1	1965; B&D
$\text{Ag}_2\text{O} \cdot \text{V}_2\text{O}_5$	3	1965; A
$\text{Ag}_2\text{O} \cdot 4\text{B}_2\text{O}_5$	4	1965; KM
$\text{AlBr}_3 \cdot \text{H}_2\text{S}$	6	1956; W,P&W
$\text{Al}_2\text{O}_3\text{C}$	7	1966; J&S
$\text{Al}_2\text{Ta}_2\text{O}_{15}(\text{F},\text{OH})$ (simgonite)	9	1962; B&B
$\text{Al}_2\text{B}_3(\text{OH})_6\text{O}_{10}$ (jeremejevite)	5	1934; G&K; 1938; S; 1955; G,B&B
$\text{Al}_2\text{C}_3\text{N}_4$	8	1953; J&W; 1966; J&W
$\text{Al}_2\text{C}_3\text{N}_4$	8	1965; J&W
$\text{Al}_2\text{C}_3\text{N}_4$	8	1963; J&W; 1966; J&W
$\text{Ba}_2\text{S}_2\text{Br}_4$	8	1958; Z
$\text{Ba}_2\text{H}_2\text{J}$	10	1965; H,B&P
$\text{Ba}_2\text{B}_2\text{O}_7$	11	1965; H,B&P
$\text{Ba}_2\text{Bi}_2\text{Nb}_2\text{O}_9$	12	1949; A
$\text{Ba}_2\text{Bi}_2\text{Ti}_2\text{O}_9$	77	1949; A; 1960; I
$\text{Ba}_2\text{TiNb}_2\text{O}_9$	13	1950; A
$\text{Ba}_2\text{TiNb}_2\text{O}_{10}$	14	1965; S
$\text{Ba}_2\text{Bi}_2\text{O}_7$	15	1948; A
$\text{Ba}_2\text{TaTiO}_5$	77	1949; A
$\text{Ba}_2\text{TiNb}_2\text{O}_9$	77	1949; A; 1960; I
$\text{Bi}_2\text{RO}_3\text{X}_2$	16	1938; S; 1939; S; 1940; S; 1941; S; S&GH; 1942; S; S&J; 1943; A; 1952; A
$\text{Ca}_2\text{B}_2\text{O}_5(\text{OH})$	17	1932; C,C&A
$\text{Ca}_2\text{Bi}_2\text{Nb}_2\text{O}_9$	77	1949; A; 1960; I
$\text{Ca}_2\text{Bi}_2\text{Ta}_2\text{O}_9$	77	1960; I
$\text{Ca}_{2.1}\text{Be}_{0.1}\text{O}_{33}$	18	1965; H&Y
$\text{Ca}_2\text{Bi}_2\text{O}_9$	15	1948; A
$\text{CdB}_2\text{O}_7$	19	1966; I&KM
$\text{Cs}_2\text{Bi}_2\text{BeAl}_2\text{O}_{18}$ (rhodizite)	20	1968; S; 1966; B&T
$\text{Cs}_2\text{Re}_2\text{Br}_11$	21	1966; E&P; 1966; E&P
$\text{Cs}_2\text{UO}_3\text{Br}_4$	22	1965; M,K&K
$\text{Cs}_2\text{UO}_4\text{Cl}_4$	23	1966; H,R&W
$\text{Cs}_2\text{RhCl}_3 \cdot \text{NH}_3\text{NO}_3$	55	1944; Z&S
$\text{Cs}_2(\text{UO}_4)\text{OCl}_3$	24	1964; A&W
$\text{CuCN} \cdot \text{Na}_2\text{H}_4$	26	1966; C,L&R
$\text{CuPb}_3\text{Sb}_2\text{S}_4$ (meneghinite)	27	1938; H; P,R&W; 1960; E&H



**Fig. XI,90a** (top). The monoclinic structure of  $Zn_2Te_3O$ , projected along its  $b$  axis.  
**Fig. XI,90b** (bottom). A packing drawing of the monoclinic structure of  $Zn_2Te_3O$ . Atoms are shown along its  $b$  axis. The zinc are the small, the tellurium the larger black circles. Atoms

# **BRIEF ATTACHMENT S**

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of

Date: March 1, 2005

Applicants: Bednorz et al.

Docket: YO987-074BZ

Serial No.: 08/479,810

Group Art Unit: 1751

Filed: June 7, 1995

Examiner: M. Kopec

For: NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION

Commissioner for Patents  
P.O. Box 1450  
Alexandria, VA 22313-1450

**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT S**

# MODERN OXIDE MATERIALS

Preparation, Properties and Device Applications

*Edited by*

**B. COCKAYNE**

*Royal Radar Establishment, Malvern, England*

and

**D. W. JONES**

*Centre for Materials Science,  
University of Birmingham, England*

1972



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formed. Both the non-polar high temperature and polar phases can be either orthorhombic and/or tetragonal. It is the single crystal form of the tungsten bronze type ferroelectric compounds which has been primarily studied for both piezoelectric and electro-optic properties.

The first compound of this crystal class reported to be ferroelectric was lead metaniobate,  $Pb_5Nb_10O_{30}$  (Goodman, 1953), with both orthorhombic  $a$  and  $b$  axes polar, an exception to the rule for these compounds. Lead metaniobate has a high Curie temperature,  $843^\circ K$ , and was developed as a piezoelectric ceramic for use over a wide temperature range.

It is an unusual material with low permittivity, moderate piezoelectric activity and very low mechanical Q. This last point is a serious drawback for many applications but is of considerable use in ultrasonic flow detection where it helps to suppress the phenomenon known as ringing.

A number of solid solutions of lead metaniobate have been studied in the polycrystalline ceramic form but the only one of any practical significance is  $(Pb_{5-x}Ba_x)Nb_{10}O_{30}$ . The optimum piezoelectric properties are found near a phase boundary occurring at  $x = 2$ , which separates two ferroelectric orthorhombic phases. Subbarao (1960) found that for  $x < 2$  the polarisation was in the  $\langle 110 \rangle$  direction whilst for  $x > 2$  the polarisation was parallel to the  $\langle 001 \rangle$  direction indicating marked influence of the highly polarisable lead ion on the polar axis. Compositions around the phase boundary possess a relatively low temperature coefficient of the resonance frequency, high mechanical Q and moderately strong piezoelectric activity which renders them suitable for resonant piezoelectric devices requiring frequency stability with temperature.

More complex compounds exhibiting the tungsten bronze structure were reported by Roth and Fang (1960), Ainger et al. (1970) and Isupov (1964). One of the more interesting compounds, barium gadolinium iron niobate,  $Ba_4Cd_2Fe_2Nb_8O_{30}$ , was reported to be a ferroelectric and ferrimagnetic ceramic, but investigations with similar ceramics showed that the weak magnetic properties were due to the presence of a second phase, barium hexaferrite.

#### C. LAYER STRUCTURE OXIDES AND COMPLEX COMPOUNDS

A large number of layer structure compounds of general formula  $(Bi_2O_2)^2+(A_{x-1}^{\text{B}}O_x)^{2-}$  have been reported (Smolenski et al. 1961; Subbarao, 1962), where A = Ca, Sr, Ba, Pb, etc., B = Ti, Nb, Ta and x = 2, 3, 4 or 5. The structure had been previously investigated by Aurivillius (1949) who described them in terms of alternate  $(Bi_2O_2)^{2+}$  layers and perovskite layers of oxygen octahedra. Few have been found to be ferroelectric and include  $SrBi_2Ta_2O_9$  ( $T_c = 583^\circ K$ ),  $PbBi_2Ta_2O_9$  ( $T_c = 703^\circ K$ ),  $BiBi_3Ti_2TaO_{12}$  or  $Bi_4Ti_3O_{12}$  ( $T_c = 948^\circ K$ ),  $Ba_2Bi_4Ti_5O_{18}$  ( $T_c = 598^\circ K$ ) and  $Pb_2Bi_4Ti_5O_{18}$  ( $T_c = 583^\circ K$ ). Only bismuth titanate  $Bi_4Ti_3O_{12}$  has been investigated in detail in the single crystal form and is finding applications in optical stores (Cummins, 1967) because of its unique ferroelectric-optical switching properties. The ceramics of other members have some interest because of their dielectric properties.

More complex compounds and solid solutions are realisable in these layer structure oxides but none have significant practical application.

formed. Both the non-polar high temperature and polar phases can be either orthorhombic and/or tetragonal. It is the single crystal form of the tungsten bronze type ferroelectric compounds which has been primarily studied for both ferroelectric and electro-optic properties.

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More complex compounds and solid solutions are realisable in these layer structure oxides but none have significant practical application.

**BRIEF ATTACHMENT T**

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of

Applicants: Bednorz et al.

Serial No.: 08/479,810

Filed: June 7, 1995

For: **NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION**

Date: March 1, 2005

Docket: YO987-074BZ

Group Art Unit: 1751

Examiner: M. Kopec

Commissioner for Patents  
P.O. Box 1450  
Alexandria, VA 22313-1450

**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT T**

# LANDOLT-BÖRNSTEIN

Numerical Data and Functional Relationships  
in Science and Technology

*New Series*

Editor in Chief: K.-H. Hellwege

Group III: Crystal and Solid State Physics

Volume 3

Ferro- and Antiferroelectric Substances

by Toshio Mitsui and

R. Abe · Y. Furuhata · K. Gesi · T. Ikeda · K. Kawabe  
Y. Makita · M. Marutake · E. Nakamura · S. Nomura  
E. Sawaguchi · Y. Shiozaki · I. Tatsuzaki · K. Toyoda

Editors: K.-H. Hellwege and A. M. Hellwege



Springer-Verlag Berlin · Heidelberg · New York 1969

## 7 Layer-structure oxides

## 7A Pure compounds of simple type

Nr. 7A-1  $\text{Bi}_3\text{TiNbO}_9$ 

1a	Dielectric anomaly associated with a phase transition was reported by ISMAILZADE in 1960.			60I1
b	phase	II	I	
	state		P <sup>a)</sup>	
	crystal system	orthorhombic <sup>b)</sup>	tetragonal <sup>b)</sup>	
	space group	Fmm2-C <sub>4v</sub> <sup>18</sup>	I4/mmm-D <sub>4h</sub> <sup>17</sup>	
	$\Theta^*$	$900 \dots 950^\circ\text{C}^b)$		
	$\rho$	$6.4 \cdot 10^3 \text{ kg m}^{-3}$		
	$a$	$a = 5.40 \text{ \AA}, b = 5.44 \text{ \AA}, c = 25.1 \text{ \AA}$ at RT.		
4	Temperature dependence of lattice parameters: Fig. 868. Linear thermal expansion: Fig. 869.			
5a	Dielectric constant: Fig. 870. $\kappa \approx 100$ at RT. The dielectric constant was not measured in the vicinity of the transition point because of high conductivity. Extrapolation of the Curie temperatures of the solid solution system obtained by the dielectric measurements indicates a transition temperature between $900^\circ$ and $950^\circ\text{C}$ for $\text{Bi}_3\text{TiNbO}_9$ .			61S11

Nr. 7A-2  $\text{Bi}_3\text{TiTaO}_9$ 

1a	Phase transition similar to that of $\text{Bi}_3\text{TiNbO}_9$ was reported by SUBBARAO in 1962.			62S17
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	space group	Fmm2-C <sub>4v</sub> <sup>18</sup>	I4/mmm-D <sub>4h</sub> <sup>17</sup>	
	$\Theta$	$870^\circ\text{C}$		
	$\rho$	$8.5 \cdot 10^3 \text{ kg m}^{-3}$		
	$a$	$a = 5.39 \text{ \AA}, b/a = 1.007, c = 25.1 \text{ \AA}$ at RT.		
4	Linear thermal expansion: see Fig. 869.			
5a	Dielectric constant: $\kappa \approx 140$ at RT.			62S17

Nr. 7A-3  $\text{CaBi}_3\text{Nb}_2\text{O}_9$ 

1a	Dielectric anomaly associated with a phase transition was discovered by ISMAILZADE in 1960.			60I1
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	space group	Fmm2-C <sub>4v</sub> <sup>18</sup>	I4/mmm-D <sub>4h</sub> <sup>17</sup>	
	$\Theta$	$625^\circ\text{C}$		
	$\rho$	$5.0 \cdot 10^3 \text{ kg m}^{-3}$		
	$a$	$a = 5.39 \text{ \AA}, b/a = 1.006, c = 25.15 \text{ \AA}$ at RT.		
4	Temperature dependence of lattice parameters: Tab. 104.			
5a	Dielectric constant: Fig. 871. $\kappa \approx 80$ at RT.			62S17

\* According to [60I1]  $\Theta$  is  $600 \dots 650^\circ\text{C}$ .

Figuren S. 376

## II 7 Oxide mit Schichtstruktur

Tab. 104. Temperature dependence of the lattice parameters of  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  and  $\text{CaBi}_4\text{Ta}_2\text{O}_9$  [60I1]

T	20	100	150	200	250	300	350	400	°C
a	5.442								
b	5.482 <sub>s</sub>	—	5.453	—	5.458	—	5.465	—	Å
c	24.920	—	5.484	—	5.487	—	5.491	—	Å
b/a	1.0075	—	24.955	—	24.990	—	25.035	—	Å
V	743.5	—	1.0056	—	1.005 <sub>s</sub>	—	1.0047	—	Å <sup>3</sup>
					748.5	—	751.0	—	
a	5.435	5.438	—	5.444	—	5.452	—	5.464	Å
b	5.468 <sub>s</sub>	5.471	—	5.475 <sub>s</sub>	—	5.479	—	5.482 <sub>s</sub>	Å
c	24.970	24.980	—	25.015	—	25.040	—	25.060	Å
b/a	1.006	1.006	—	1.005 <sub>s</sub>	—	1.005	—	1.003 <sub>s</sub>	Å
V	742.0	743.2	—	745.6	—	748.0	—	750.6	Å <sup>3</sup>
T	450	500	550	575	600	650	700	—	°C
a	5.480	5.485	5.488 <sub>s</sub>	5.495 <sub>s</sub>	—	5.502 <sub>s</sub>	5.504	Å	
b	5.496 <sub>s</sub>	5.501 <sub>s</sub>	5.502 <sub>s</sub>	5.503 <sub>s</sub>	—	5.502 <sub>s</sub>	5.504	Å	
c	25.070	25.080	25.090	25.105	—	25.125	25.140	Å	
b/a	1.0036	1.0029	1.0025	1.0015	—	1.000	1.000	—	
V	755.0	756.8	758.0	759.3	—	760.7	761.6	Å <sup>3</sup>	
a	—	5.470	5.473	—	5.479	5.484	—	Å	
b	—	5.483 <sub>s</sub>	5.484	—	5.479	5.484	—	Å	
c	—	25.070	25.083	—	25.085	25.105	—	Å	
b/a	—	1.002 <sub>s</sub>	1.002 <sub>s</sub>	—	1.000	1.000	—	—	
V	—	751.9	752.8	—	730.0	755.0	—	Å <sup>3</sup>	

Nr. 7A-4  $\text{CaBi}_4\text{Ta}_2\text{O}_9$ 

1a	Dielectric anomaly associated with a phase transition was discovered by ISMAILZADE in 1960.	60I1
b	phase state crystal system space group $\Theta$	II I orthorhombic tetragonal Fmm2-C <sub>4v</sub> <sup>18</sup> I4/mmm-D <sub>4h</sub> <sup>17</sup>
		575 °C
	$\epsilon = 7.5 \cdot 10^3 \text{ kg m}^{-3}$ , $a = 5.428 \text{ Å}$ , $b/a = 1.006$ , $c = 24.90 \text{ Å}$ at RT.	60I1 61S11
4	Temperature dependence of lattice parameter: see Tab. 104.	
5a	Dielectric constant: Fig. 872.	

Nr. 7A-5  $\text{SrBi}_4\text{Nb}_2\text{O}_9$ 

1a	Dielectric anomaly associated with a phase transition was discovered by SMOLENSKII in 1961.	61S11
b	phase state crystal system $\Theta$	II I orthorhombic tetragonal
		420 440 <sup>a</sup> ) °C
	$\epsilon = 6.9 \cdot 10^3 \text{ kg m}^{-3}$ , $a = 5.506 \text{ Å}$ , $b/a = 1.000$ , $c = 25.05 \text{ Å}$ at RT.	61S11 *)62S17
5a	Dielectric constant: Fig. 873. $\propto \approx 190$ at RT. $\propto = C/(T - \Theta_p)$ , where $C = 0.55 \cdot 10^5 \text{ °C}$ , $\Theta_p = 390 \text{ °C}$ .	62S15
7a	Piezoelectricity: $d_{33} = 1.0 \cdot 10^{-11} \text{ C N}^{-1}$ .	62S17 62S17

Nr. 7A-6  $\text{SrBi}_2\text{Ta}_2\text{O}_9$ 

1a	Ferroelectricity in $\text{SrBi}_2\text{Ta}_2\text{O}_9$ was reported by SMOLENSKII in 1961.			
b	phase	II	I	
	state	F	P	
	crystal system	orthorhombic	tetragonal	
	$\Theta$	310 °C		
	$\rho$	$7.5 \cdot 10^8 \text{ kg m}^{-3}$		61S11
	$a$	$5.512 \text{ \AA}$ , $b/a = 1.000$ , $c = 25.00 \text{ \AA}$ at RT.		62S15
5a	Dielectric constant: Fig. 874. $\kappa \approx 180$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 2.0 \cdot 10^8 \text{ ^\circ C}$ , $\Theta_p = 190 \text{ ^\circ C}$ .			62S17
c	Spontaneous polarization: $P_s = 5.8 \cdot 10^{-2} \text{ C m}^{-2}$ at 25 °C.			62S17
7a	Piezoelectric constant: $d_{33} = 2.3 \cdot 10^{-11} \text{ C N}^{-1}$ .			62S17

Nr. 7A-7  $\text{BaBi}_2\text{Nb}_2\text{O}_9$ 

1a	Dielectric anomaly associated with a phase transition was discovered by SMOLENSKII in 1961.			61S11
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	$\Theta$	210 °C		61S11
		200°) °C		62S17
	$\rho$	$6.3 \cdot 10^8 \text{ kg m}^{-3}$		
	$a$	$5.554 \text{ \AA}$ , $b/a = 1.000$ , $c = 25.60 \text{ \AA}$ at RT.		62S15
5a	Dielectric constant: Fig. 875. $\kappa = 280$ at RT.			62S17

Nr. 7A-8  $\text{BaBi}_2\text{Ta}_2\text{O}_9$ 

1a	Dielectric anomaly associated with a phase transition was discovered by SMOLENSKII in 1961.			61S11
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	$\Theta$	110°) °C		61S11
	According to [61S11] $\Theta$ is 70 °C.			61S11
	$\rho$	$8.4 \cdot 10^8 \text{ kg m}^{-3}$		
	$a$	$5.556 \text{ \AA}$ , $b/a = 1.000$ , $c = 25.50 \text{ \AA}$ at RT.		62S15
5a	Dielectric constant: Fig. 876. $\kappa = 400$ at RT.			62S17

Nr. 7A-9  $\text{PbBi}_2\text{Nb}_2\text{O}_9$ 

1a	Dielectric anomaly associated with a phase transition in $\text{PbBi}_2\text{Nb}_2\text{O}_9$ was reported by SMOLENSKII in 1959.			59S8
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	$\Theta$	526 °C		59S8
		550°) °C		61S15
	$\rho$	$7.6 \cdot 10^8 \text{ kg m}^{-3}$		
	$a$	$5.488 \text{ \AA}$ , $b/a = 1.002$ , $c = 25.55 \text{ \AA}$ at RT.		62S15
3	Crystal structure: Fig. 877.			
4	Temperature dependence of lattice parameters: Fig. 878.			
5a	Dielectric constant: Fig. 879. $\kappa = 170$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 1.3 \cdot 10^8 \text{ K}$ , $\Theta_p = 510 \text{ °C}$ .			62S17
7a	Piezoelectric constant: $d_{33} = 1.5 \cdot 10^{-11} \text{ C N}^{-1}$ .			62S17

Nr. 7A-10  $\text{PbBi}_2\text{Ta}_2\text{O}_9$ 

1a b	Ferroelectricity was reported by SUBBARAO <sup>a)</sup> and SMOLENSKIR <sup>b)</sup> independently in 1961.			<sup>a)</sup> 61S15 <sup>b)</sup> 61S11
phase	II	I		
state	F	P		
crystal system	orthorhombic	tetragonal		
$\Theta$	430 °C			61S15
$\rho = 9.0 \cdot 10^3 \text{ kg m}^{-3}$ .				61S11
$a = 5.496 \text{ \AA}$ , $b/a = 1.000$ , $c = 25.40 \text{ \AA}$ at RT.				62S15
5a	Dielectric constant: Fig. 880. $\kappa = 180$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 3.7 \cdot 10^4 \text{ ^\circ C}$ , $\Theta_p = 325 \text{ ^\circ C}$ .			62S17
7a	Piezoelectric constant: $d_{33} = 5 \cdot 10^{-12} \text{ C N}^{-1}$ .			62S17

Nr. 7A-11  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ 

1a b	Ferroelectricity in $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ was reported by VAN UITER <sup>a)</sup> et al. in 1961.			61V2
phase	II	I		
state	F	P		
crystal system	monoclinic <sup>a)</sup> (pseudo-orthorhombic)	tetragonal		61V2 <sup>a)</sup> 67C6
$\Theta$	675 °C			
Unit cell is very nearly orthorhombic with the lattice parameters: $a_{\text{orth}} = 5.411 \text{ \AA}$ , $b_{\text{orth}} = 5.448 \text{ \AA}$ , $c_{\text{orth}} = 32.85 \text{ \AA}$ at RT. Relations between crystallographic axes: Fig. 881. $P_s$ lies in a direction tilted at approximately 7° (or less) from the major crystal surface in a plane parallel to the pseudo-orthorhombic $b - c$ plane.			67C6	
2a	Crystal growth: Cooling method from melt consisting of 100 $\text{Bi}_4\text{O}_7$ and 5 $\text{TiO}_3$ (weight ratio).			61V2
3	Crystal structure: Fig. 882.			
4	Temperature dependence of lattice parameter: Fig. 883. Thermal expansion: Fig. 884.			
5a c	Dielectric constant: Fig. 885. $P_s$ and $E_c$ : Fig. 886, 887. TAMBOVITSEV et al. measured $P_s$ and $E_c$ by applying a field parallel to the $c_{\text{orth}}$ direction, $P_s = 1.99 \cdot 10^{-8} \text{ C m}^{-2}$ , $E_c = 1.13 \cdot 10^4 \text{ V m}^{-1}$ . According to [67C6], the spontaneous polarization lies in the pseudo-orthorhombic (100) plane and has a value larger than $30 \cdot 10^{-8} \text{ C m}^{-2}$ .			63T1 67C6
7	Piezoelectric constant: $d_{33} = 2.0 \cdot 10^{-11} \text{ C N}^{-1}$ .			61S17
10	Conductivity: see			64P3
14a b	Domain structure: see Domains have been observed by polarized light. Switching: Fig. 888, 889. See also Fig. 892, Tab. 105 and:			64P3 66C7
17	Twinning structure: see			66P6 64P3

Nr. 7A-12  $\text{BaBi}_4\text{Ti}_3\text{NbO}_{12}$ 

1a b	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1961.			61S15
phase	II	I		
state		P		
crystal system	pseudo-tetragonal	tetragonal		
$\Theta$	270 °C			61S15

Nr. 7A-13  $\text{PbBi}_4\text{Ti}_3\text{NbO}_{12}$ 

1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1961.	61S15
* Point group is m.		

1b	phase	II	I		
	state		P		
	crystal system	pseudo-tetragonal	tetragonal		
	$\Theta$	290 °C			
	$a = 3.687 \text{ \AA}$ , $c = 33.55 \text{ \AA}$ at RT.			61S15 61S15	
<b>Nr. 7A-14 BaBi<sub>4</sub>Ti<sub>4</sub>O<sub>15</sub></b>					
1a	Dielectric anomaly associated with a phase transition was reported independently by SUBBARAO <sup>a)</sup> and by SMOLENSKII <sup>b)</sup> in 1961. Ferroelectric activity was reported independently by FANG et al. in 1961 <sup>c)</sup> .				
b	phase	II	I		
	state	F	P		
	crystal system	orthorhombic (or pseudo-orthorhombic)	tetragonal		
	$\Theta$	375 °C 395 <sup>a)</sup> °C			
	$\rho = 5.7 \cdot 10^8 \text{ kg m}^{-3}$ $a = 5.461 \text{ \AA}$ , $b/a = 1.000$ , $c = 41.85 \text{ \AA}$ at RT.			<sup>a)</sup> 61S15 62S15	
3	Crystal structure: Fig. 890.				
5a	Dielectric constant: Fig. 891. $\kappa = 150$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 2.5 \cdot 10^5 \text{ }^\circ\text{K}$ , $\Theta_p = 335 \text{ }^\circ\text{C}$ .				
7a	Piezoelectric constant: $d_{33} = 2.3 \cdot 10^{-11} \text{ C N}^{-1}$ .				
14b	Switching: Fig. 892; Tab. 105.				
Tab. 105. BaBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub> , Ba <sub>2</sub> Bi <sub>4</sub> Ti <sub>5</sub> O <sub>18</sub> , Bi <sub>4</sub> Ti <sub>5</sub> O <sub>18</sub> , BaTiO <sub>3</sub> (for comparison). Switching parameters in comparison with those of BaTiO <sub>3</sub> [62F1]. $t_s = t_{\infty} \exp(+\alpha/E)$ , $t_s$ = switching time					
	BaTiO <sub>3</sub>	Bi <sub>4</sub> Ti <sub>5</sub> O <sub>18</sub>	BaBi <sub>4</sub> Ti <sub>4</sub> O <sub>15</sub>	Ba <sub>2</sub> Bi <sub>4</sub> Ti <sub>5</sub> O <sub>18</sub>	
$\alpha$	6.1	41	23	76	$10^6 \text{ V m}^{-1}$
$t_{\infty}$	0.4	$10^{-2}$	1.5	$10^{-3}$	$\mu \text{ sec}$
<b>Nr. 7A-15 PbBi<sub>4</sub>Ti<sub>4</sub>O<sub>15</sub></b>					
1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1961.				61S15
b	phase	II	I		
	state		P		
	crystal system	orthorhombic (possibly)	tetragonal		
	$\Theta$	570 °C			
	$\rho = 6.6 \cdot 10^8 \text{ kg m}^{-3}$ $a = 5.437 \text{ \AA}$ , $b/a = 1.000$ , $c = 41.35 \text{ \AA}$ at RT.				62S15
5a	Dielectric constant: Fig. 893. $\kappa = 220$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 1.4 \cdot 10^5 \text{ }^\circ\text{C}$ , $\Theta_p = 552 \text{ }^\circ\text{C}$ .				61S15 62S17
7a	Piezoelectric constant: $d_{33} = 2.3 \cdot 10^{-11} \text{ C N}^{-1}$ .				62S17
<b>Nr. 7A-16 SrBi<sub>4</sub>Ti<sub>4</sub>O<sub>15</sub></b>					
1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1961.				61S15
b	phase	II	I		
	state		P		
	crystal system	orthorhombic (possibly)	tetragonal		
	$\Theta$	530 °C			
	$\rho = 5.2 \cdot 10^8 \text{ kg m}^{-3}$ $a = 5.428 \text{ \AA}$ , $b/a = 1.000$ , $c = 40.95 \text{ \AA}$ at RT.				62S17 62S15
5a	Dielectric constant: Fig. 894. $\kappa = 190$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 0.68 \cdot 10^5 \text{ }^\circ\text{C}$ , $\Theta_p = 485 \text{ }^\circ\text{C}$ .				62S17
7a	Piezoelectric constant: $d_{33} = 1.5 \cdot 10^{-12} \text{ C N}^{-1}$ .				62S17

Nr. 7A-17  $\text{CaBi}_4\text{Ti}_4\text{O}_{15}$ 

1a	$\text{CaBi}_4\text{Ti}_4\text{O}_{15}$ was investigated by SUBBARAO in 1962. No dielectric anomaly has been detected.	62S17 62S15
b	Orthorhombic: $a = 5.418 \text{ \AA}$ , $b/a = 1.002$ , $c = 40.75 \text{ \AA}$ at RT. $\rho = 4.7 \cdot 10^3 \text{ kg m}^{-3}$ .	
5a	Dielectric constant: Fig. 895. $\kappa = 120$ at RT.	61S11

Nr. 7A-18  $\text{Bi}_5\text{Ti}_2\text{GaO}_{15}$ 

1a	$\text{Bi}_5\text{Ti}_2\text{GaO}_{15}$ was investigated by SUBBARAO in 1962. No dielectric anomaly has been detected.	62S17 62S15
b	Orthorhombic: $a = 5.408 \text{ \AA}$ , $b/a = 1.006$ , $c = 41.05 \text{ \AA}$ at RT. $\rho = 7.3 \cdot 10^3 \text{ kg m}^{-3}$ .	
5a	Dielectric constant: $\kappa = 150$ at RT.	62S17

Nr. 7A-19  $\text{Ba}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ 

1a	Ferroelectric activity of $\text{Ba}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ was observed by AURIVILLIUS in 1962.	62A5
b	phase                    II                    I state                    F                    P crystal system            orthorhombic        tetragonal $\Theta$ 325 °C $a = 5.527 \text{ \AA}$ , $b = 5.514 \text{ \AA}$ , $c = 50.37 \text{ \AA}$ at RT.	
3	Crystal structure: Fig. 896; Tab. 106.	62A5 6315
4	Temperature dependence of lattice parameter: Fig. 897.	
5a	Dielectric constant: Fig. 898. $\kappa' = 360$ , $\kappa'' = 22$ at RT.	
c	Remanent polarization: $P_r = 2 \cdot 10^{-4} \text{ C m}^{-2}$ at RT. Coercive field: $E_c = 1.0 \cdot 10^3 \text{ V m}^{-1}$ at RT.	62A5 62A5
14b	Switching: see Fig. 892; Tab. 105.	

Tab. 106.  $\text{Ba}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ . Fractional coordinates of atoms [62A5]. Space group of I4/mmm was assumed.

I4/mmm	(0, 0, 0; 1/2, 1/2, 1/2) +	
4 Bi      in 4(e):	$\pm 0, 0, z$ :	$z = 0.2255$
4 (Bi, Ba) in 4(e):		$z = 0.0420$
4 (Bi, Ba) in 4(e):		$z = 0.1300$
2 Ti      in 2(b):	$\pm 0, 0, 1/2$	
4 Ti      in 4(e):		$z = 0.3370$
4 Ti      in 4(e):		$z = 0.4185$
4 O      in 4(c):	$0, 1/2, 0; 1/2, 0, 0$	
4 O      in 4(d):	$0, 1/2, 1/4; 1/2, 0, 1/4$	
4 O      in 4(e):		$z = 0.2962$
4 O      in 4(e):		$z = 0.3378$
4 O      in 4(e):		$z = 0.4593$
8 O      in 8(g):	$\pm (0, 1/2, z; 1/2, 0, z)$	$z = 0.0815$
8 O      in 8(g):		$z = 0.1630$

Nr. 7A-20  $\text{Pb}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ 

1a	Ferroelectric activity in $\text{Pb}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ was observed by SUBBARAO in 1962.	62S17
b	phase                    II                    I state                    F                    P crystal system            orthorhombic        tetragonal $\Theta$ 310 °C $\rho = 6.6 \cdot 10^3 \text{ kg m}^{-3}$ . $a = 5.461 \text{ \AA}$ , $b/a = 1.000$ , $c = 49.70 \text{ \AA}$ at RT.	
		62S17
		62S15

5a	Dielectric constant: Fig. 899. $\chi = 400$ at RT. $\chi = C/(T - \Theta_p)$ , $C = 4.1 \cdot 10^5 \text{ K}$ , $\Theta_p = 280 \text{ }^\circ\text{C}$ .			62S17
c	Spontaneous polarization: $P_s = 6 \cdot 10^{-2} \text{ C m}^{-2}$ at $235 \text{ }^\circ\text{C}$ .			62S17
7a	Piezoelectric constant: $d_{33} = 2.5 \cdot 10^{-12} \text{ C N}^{-1}$ .			62S17
<b>Nr. 7A-21 <math>\text{Sr}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}</math></b>				
1a	Ferroelectric activity in $\text{Sr}_2\text{Bi}_4\text{Ti}_5\text{O}_{18}$ was observed by SUBBARAO in 1962.			62S17
b	phase	II	I	
	state	F	P	
	crystal system	orthorhombic (possibly)	tetragonal	
	$\Theta$	$285 \text{ }^\circ\text{C}$		
		$\rho = 5.3 \cdot 10^3 \text{ kg m}^{-3}$ ,		
		$a = 5.461 \text{ \AA}$ , $b/a = 1.000$ , $c = 48.80 \text{ \AA}$ at RT.		
5a	Dielectric constant: Fig. 900. $\chi = 280$ at RT. $\chi = C/(T - \Theta_p)$ , $C = 0.47 \cdot 10^5 \text{ K}$ , $\Theta_p = 255 \text{ }^\circ\text{C}$ .			62S17
c	Spontaneous polarization: $P_s = 3.5 \cdot 10^{-2} \text{ C m}^{-2}$ at $255 \text{ }^\circ\text{C}$ .			62S17
7a	Piezoelectric constant: $d_{33} = 2.5 \cdot 10^{-12} \text{ C N}^{-1}$ .			62S17
<b>Nr. 7A-22 <math>\text{Bi}_4\text{Ti}_5\text{O}_{11}</math></b>				
1a	Dielectric anomaly associated with a phase transition was observed in $\text{Bi}_4\text{Ti}_5\text{O}_{11}$ by SUBBARAO in 1962.			62S16
b	phase	III	II	I
	crystal system	monoclinic	monoclinic	
	space group	$\text{C}2/\text{c}-\text{C}_{\text{sh}}^6$	$\text{C}2/\text{m}-\text{C}_{\text{sh}}^{**}$	
	$\Theta$	$250^a)$ $1200^a)$ ${}^\circ\text{C}$		
		$\rho = (6.12 \pm 0.02) \cdot 10^3 \text{ kg m}^{-3}$ ,		
		$a = (14.612 \pm 0.006) \text{ \AA}$ , $b = (3.799 \pm 0.004) \text{ \AA}$ , $c = (14.946 \pm 0.006) \text{ \AA}$ ,		
		$\beta = (93.13 \pm 0.01) {}^\circ$ at RT.		
3	Crystal structure: $Z = 2$ in phase II. $Z = 4$ in phase III. Fig. 901, 902; Tab. 107.			65J4
4	Thermal expansion: Fig. 903.			
5a	Dielectric constant: Fig. 904.			
c	No hysteresis loops could be obtained between $25 \text{ }^\circ\text{C}$ and $290 \text{ }^\circ\text{C}$ .			62S16
Tab. 107. $\text{Bi}_4\text{Ti}_5\text{O}_{11}$ . Atomic parameters at RT [65J4]				
Atom	x	y	z	
O(1)	0.0	0.262	$\pm 0.012$	0.250
O(2)	$0.1828 \pm 0.0024$	0.246	$\pm 0.007$	$0.2207 \pm 0.0024$
O(3)	$0.1408 \pm 0.0024$	0.256	$\pm 0.007$	$0.0338 \pm 0.0024$
O(4)	$0.0814 \pm 0.0024$	0.760	$\pm 0.007$	$0.1259 \pm 0.0024$
O(5)	$0.2662 \pm 0.0024$	0.747	$\pm 0.007$	$0.0880 \pm 0.0024$
O(6)	$0.0546 \pm 0.0024$	0.770	$\pm 0.007$	$0.9221 \pm 0.0024$
Ti(1)	$0.0530 \pm 0.0006$	0.250	$\pm 0.002$	$0.1406 \pm 0.0006$
Ti(2)	$0.1461 \pm 0.0006$	0.759	$\pm 0.002$	$0.0162 \pm 0.0006$
Bi	$0.3211 \pm 0.00015$	0.1747	$\pm 0.0005$	$0.1798 \pm 0.00015$

Thermal parameter  $B = 0.33 \text{ \AA}^2$  for all atoms. Coordinates and standard deviations in cell fractions.

### 7B Complex compounds and solid solutions

**Nr. 7B-1  $\text{Bi}_{4-x}\text{Me}^{3+}_x\text{Ti}_{1-x}\text{Nb}_{1+x}\text{O}_9$  ( $\text{Me}^{3+} = \text{Ba}, \text{Sr}, \text{Pb}$ )**

1b Lattice parameter: Fig. 905.  
Transition temperature: Fig. 906.

5 Dielectric constant: Fig. 907.

**Nr. 7B-2  $\text{Bi}_{4-x}\text{Me}^{3+}_x\text{Ti}_{1-x}\text{Nb}_x\text{O}_{12}$  ( $\text{Me}^{3+} = \text{Ba}, \text{Sr}, \text{Pb}$ )**

1b Lattice parameter: Fig. 908.  
Transition temperature: Fig. 909.

5 Dielectric constant: Fig. 910.

\* The unit cell of phase II has about half the volume of the unit cell of phase III.

Nr. 7B-3 $\text{Na}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$				
1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1962.			
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	$\Theta$	650 °C		62S17
	$\rho = 6.3 \cdot 10^8 \text{ kg m}^{-3}$ .			62S15
	$a = 5.427 \text{ Å}, b/a = 1.006, c = 40.65 \text{ Å}$ at RT.			
5a	Dielectric constant: Fig. 911. $\kappa = 200$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 0.79 \cdot 10^5 \text{ °K}$ , $\Theta_p = 610 \text{ °C}$ .			
7a	Piezoelectric constant: $d_{33} = 1.0 \cdot 10^{-11} \text{ C N}^{-1}$ .			
Nr. 7B-4 $\text{K}_{0.5}\text{Bi}_{4.5}\text{Ti}_4\text{O}_{15}$				
1a	Dielectric anomaly associated with a phase transition was reported by SUBBARAO in 1962.			
b	phase	II	I	
	state		P	
	crystal system	orthorhombic	tetragonal	
	$\Theta$	550 °C		62S17
	$\rho = 6.7 \cdot 10^8 \text{ kg m}^{-3}$ .			62S15
	$a = 5.440 \text{ Å}, b/a = 1.004, c = 41.15 \text{ Å}$ at RT.			
5a	Dielectric constant: Fig. 912. $\kappa = 140$ at RT. $\kappa = C/(T - \Theta_p)$ , $C = 0.74 \cdot 10^5 \text{ °K}$ , $\Theta_p = 515 \text{ °C}$ .			
7a	Piezoelectric constant: $d_{33} = 1.0 \cdot 10^{-11} \text{ C N}^{-1}$ .			
Nr. 7B-5 $(\text{Pb}_{1-x}\text{Ba}_x)\text{Bi}_4\text{Nb}_3\text{O}_9$ and $(\text{Pb}_{1-x}\text{Sr}_x)\text{Bi}_4\text{Nb}_3\text{O}_9$				
1b	Transition temperature: Fig. 913.			
5	Dielectric constant: Fig. 914.			
Nr. 7B-6 $(1-x)\text{Bi}_4\text{Ti}_4\text{O}_{15} - x\text{BaTiO}_3$				
5	Transition temperature: Fig. 915.			
Nr. 7B-7 $\text{Bi}_{4+x}\text{Pb}_{1-x}\text{Ti}_{4-x}\text{Ga}_x\text{O}_{15}$				
1a	Another formula for this solid solution is $(1 - x)\text{PbBi}_4\text{Ti}_4\text{O}_{15} + x\text{Bi}_4\text{Ti}_3\text{GaO}_{15}$ . Properties of this solid solution were studied by SUBBARAO in 1962.			
b	$x = 0.25$ :			
	phase	II	I	
	state		P	
	crystal system	orthorhombic (pseudo-tetragonal)	tetragonal	
	$\Theta$	600 °C		
	Pseudo-tetragonal cell parameter: $a = 3.842 \text{ Å}, c = 41.40 \text{ Å}$ at RT. Dielectric constant: $\kappa = 180$ at RT; $\kappa = 3035$ at $\Theta$ .			
	$x = 0.5$ :			
	phase	II	I	
	state		P	
	crystal system	orthorhombic (pseudo-tetragonal)	tetragonal	
	$\Theta$	620 °C		
	Pseudo-tetragonal cell parameter: $a = 3.842 \text{ Å}, c = 41.40 \text{ Å}$ at RT. Dielectric constant: $\kappa = 179$ at RT; $\kappa = 1930$ at $\Theta$ .			

**BRIEF ATTACHMENT U**

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of

Date: March 1, 2005

Applicants: Bednorz et al.

Docket: YO987-074BZ

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Filed: June 7, 1995

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For: NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION

Commissioner for Patents  
P.O. Box 1450  
Alexandria, VA 22313-1450

**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT U**

# STRUCTURE, PROPERTIES AND PREPARATION OF PEROVSKITE-TYPE COMPOUNDS

BY  
**FRANCIS S. GALASSO**  
*United Aircraft Research Laboratories*

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EXD-EX



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**BRIEF ATTACHMENT V**

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of

Applicants: Bednorz et al.

Serial No.: 08/479,810

Filed: June 7, 1995

For: NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION

Date: March 1, 2005

Docket: YO987-074BZ

Group Art Unit: 1751

Examiner: M. Kopeć

Commissioner for Patents  
P.O. Box 1450  
Alexandria, VA 22313-1450

**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT V**

## ARKIV FÖR KEMI Band 1 nr 54

Communicated 15 September 1949 by ARNE WESTGREN and ARNE TIBELIUS

## Mixed bismuth oxides with layer lattices

I. The structure type of  $\text{CaNb}_2\text{Bi}_2\text{O}_9$ 

By BENGT AURIVILLIUS

With 5 figures in the text

In the course of a comprehensive investigation of mixed bismuth oxides, the system  $\text{Bi}_2\text{O}_3 - \text{TiO}_2$  was studied. At about 40 atomic % of  $\text{TiO}_2$  a phase with a body-centered pseudo-tetragonal unit cell with  $a = 3.84$  and  $c = 32.8 \text{ \AA}$  was found. X-ray analysis (to be published later) seemed to show that the structure was built up of  $\text{Bi}_2\text{O}_2^{2+}$  layers parallel to the basal plane, and sheets of composition  $\text{Bi}_2\text{Ti}_3\text{O}_{10}^{2-}$ . The atomic arrangement within the  $\text{Bi}_2\text{Ti}_3\text{O}_{10}^{2-}$  sheets seemed to be the same as in structures of the perowskite type and the structure could then be described as consisting of  $\text{Bi}_2\text{O}_2^{2+}$  layers between which double perowskite layers are inserted.

An attempt was then made to synthesize compounds where the  $\text{Bi}_2\text{O}_2^{2+}$  layers alternate with single perowskite layers. The general formula for such compounds could be expected to be:  $(\text{MeBi})_6\text{R}_4\text{O}_{18}$ . In actual fact compounds with this structure could be prepared with Me: Na K Ca Ba Sr Pb R: Ti Nb Ta.

Procedure: Weighed amounts of the appropriate oxides or carbonates were mixed and heated in platinum or gold crucibles to about  $1000^\circ\text{C}$ . A number of compounds with the general formula  $(\text{Bi, Me})_6\text{R}_4\text{O}_{18}$  were prepared. Out of these the following were found to have a body-centered tetragonal or pseudo-tetragonal unit cell. The real unit cells, however, appeared to be face-centered-orthorhombic.

Composition	Orthorhombic description			Pseudo-tetragonal description	
	<i>a</i>	<i>b</i>	<i>c</i>	<i>a</i>	<i>c</i>
$\text{Bi}_3\text{NbTiO}_9$ . . . . .	5.405	5.442	25.11	3.836	25.11
$\text{Bi}_3\text{TaTiO}_9$ . . . . .	5.402	5.436	25.15	3.832	25.15
$\text{CaBi}_2\text{Nb}_2\text{O}_9$ . . . . .	5.435	5.485	24.87	3.860	24.87
$\text{SrBi}_2\text{Nb}_2\text{O}_9$ . . . . .	5.504	5.504	25.05	3.892	25.05
$\text{SrBi}_2\text{Ta}_2\text{O}_9$ . . . . .	5.509	5.509	25.06	3.895	25.06
$\text{BaBi}_2\text{Nb}_2\text{O}_9$ . . . . .	5.533	5.533	25.55	3.912	25.55
$\text{PbBi}_2\text{Nb}_2\text{O}_9$ . . . . .	5.492	5.503	25.53	3.887	25.53
$\text{KBi}_5\text{Nb}_4\text{O}_{18}$ . . . . .	5.506	5.506	25.26	3.893	25.26
$\text{NaBi}_5\text{Nb}_4\text{O}_{18}$ . . . . .	5.47	5.47	26.94	3.87	26.94

B. AURIVILLIUS, *Mixed bismuth oxides with layer lattices*

Single crystals were prepared from the  $\text{PbBi}_2\text{Nb}_2\text{O}_9$  and  $\text{Bi}_2\text{NbTiO}_9$  phases. Weissenberg photographs of  $0kl$  and  $1kl$  (pseudo-tetragonal cell) were taken. In the powder photographs of  $\text{Bi}_2\text{NbTiO}_9$  (Table 6a) the reflections  $110$ ,  $211$ ,  $215$ ,  $220$  and  $310$  were clearly split up. No cleavage was found for the reflections  $10l$ ,  $20l$ , and  $30l$ , (in all cases pseudo-tetragonal indices). From this it was concluded that the structure might be described by means of orthorhombic unit cells, having the same  $c$  axes as the pseudo-tetragonal cells, and  $a$  and  $b$  axes equal to the diagonals of the pseudo-tetragonal cells. Using orthorhombic units the Weissenberg photographs register  $hkl$  and  $h, h+2, l$ . In Table 6a the  $\sin^2 \theta$  of  $\text{Bi}_2\text{NbTiO}_9$  are calculated on the assumption of an orthorhombic unit cell.

A few discrepancies occur between the intensities of the spots as found in the Weissenberg photographs (first layer) and in the powder photographs. In the Weissenberg photographs ( $h, h+2, l$ ), no difference was found between reflections  $hkl$  and  $khl$ . From the powder photographs it is seen that  $024$  might be  $< 204$  and that  $311 < 131$  and  $3111 < 1311$ . The reason might be the orientation of the powder.

 $\text{PbBi}_2\text{Nb}_2\text{O}_9$  phase

The powder photographs of  $\text{PbBi}_2\text{Nb}_2\text{O}_9$  (Table 6b) could be explained assuming a tetragonal cell with  $a = 3.887 \text{ \AA}$  and  $c = 25.53 \text{ \AA}$ , but for two lines being split up, which indicated an orthorhombic unit cell with axes  $a = 5.492$ ,  $b = 5.503$  and  $c = 25.53 \text{ \AA}$ . As in  $\text{Bi}_2\text{NbTiO}_9$ , it was thus assumed that the real symmetry is  $D_{2h} - mmm$ , though nothing in the Weissenberg photographs indicated a lower Laue symmetry than  $D_{2h} - 4/mmm$ . The observed density was 7.91, thus allowing 4 formula units/unit cell ( $d_{\text{calc.}} = 8.22$ ).

With the exception of the criterion for face-centering that  $hkl$  occurring only with  $h, k, l$  all odd or all even, no systematic extinctions were found. This is characteristic of the space groups  $D_{2h}^{22}$ ,  $D_2'$  and  $C_{2h}^{18}$ .

## Positions of the metal atoms

As the scattering factors for the Pb and the Bi atoms are almost the same, it makes no difference in the intensity calculations whether the Pb and the Bi atoms occupy separate positions or are mixed at random. Therefore no difference will be made between Pb and Bi; they will both be denoted by Me.

The intensities of the reflections seemed to depend mainly on the value of  $l$  (see Table 1a). It therefore seemed probable that at least the Me and the Nb atoms are placed along the lines:  $(000; \frac{1}{2} \frac{1}{2} 0; \frac{1}{2} 0 \frac{1}{2}; 0 \frac{1}{2} \frac{1}{2}) + 00z$ . The sum of  $\sum_i I_{00i} \cos 2\pi lz$  and  $\sum_i I_{11i} \cos 2\pi lz$  will under such conditions represent the Patterson function along  $00z$ . In Fig. 1a these sums are plotted as functions of  $z$ . It is seen from the graph that high maxima occur for  $z = 0.20$  and  $z = 0.40$ .

The unit cell of  $\text{PbBi}_2\text{Nb}_2\text{O}_9$  contains 12 Me atoms and 8 Nb atoms.

If the space groups are assumed to be  $D_{2h}^{22}$ ,  $D_2'$  or  $C_{2h}^{18}$  a or  $b$ , the only way of placing 12 Me atoms on the lines  $00z$  is in one 4-fold and one 8-fold position. With these assumptions the only 4-fold positions possible are  $000$  or  $00\frac{1}{2}$ .

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Table 1a

Weissenberg Photographs of  $PbBi_2Nb_2O_9$ . Cu  $K\alpha$  radiation

The crystals form very thin plates, and therefore considerable absorption occurs. Spots in the vicinity of the lines described by WELLS (2) will therefore be weakened. The regions of maximum absorption are denoted by dotted lines. In the tables 1, 2 and 3 pseudo-tetragonal indices are used, and observed and calculated intensities for the reflections: 00 $\bar{l}$ , 10 $\bar{l}$ , 11 $\bar{l}$ , 20 $\bar{l}$ , and 21 $\bar{l}$  are given. With orthorhombic description these reflections would have been denoted by: 00 $\bar{l}$ , 02 $\bar{l}$  or 20 $\bar{l}$ , 22 $\bar{l}$ , 13 $\bar{l}$  or 31 $\bar{l}$ .

$l$	$I_1$	$I_2$	$I_{00\bar{l}}$	$\frac{I_{obs.}}{I_{11\bar{l}}}$	$I_{20\bar{l}}$
2	18	1.2			
4	9.0	34	m-	m	w
6	0.1	8.4	vvw	m	—
8	25	14	m-	w	w-
10	350	340	vst	m+	m
12	19	0.2	w	—	—
14	36	100	m+	vvw	w-
16	9.6	4.8	vw	—	—
18	45	31	m	w	w
20	280	230	st	m+	m+
22	22	0.04	—	—	—
24	71	200	m+	m	m+
26	27	14	w-	vvw	vw
28	85	26	m-	w	w
30	190	130	m	m	
32	25	8.4	w		
$l$	$I_1$	$I_2$	$I_{10\bar{l}}$	$\frac{I_{obs.}}{I_{21\bar{l}}}$	
1	1.7	17	m-	—	
3	20	6.3	m-	vvw	
5	380	370	vst	st	
7	18	0.0	—	—	
9	12	63	m	w	
11	3.2	5.8	—	—	
13	32	23	w	vvw	
15	320	280	st	w	
17	20	0.2	—	—	
19	55	160	m+	w+	
21	18	7.8	vvw	—	
23	61	32	m	w+	
25	230	170	m+	m	
27	24	1.7	—	—	
29	85	250	m+		
31	48	23	w		

B. AURIVILLIUS, *Mixed bismuth oxides with layer lattices*

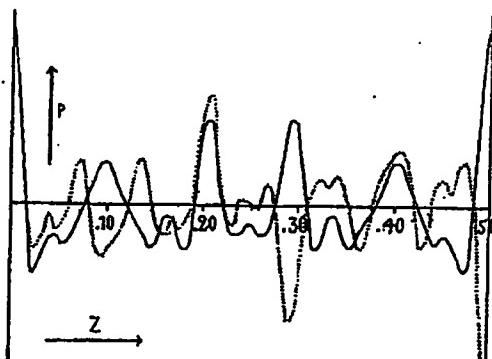
*Table 1b*  
Weissenberg Photographs of  $PbBi_2Nb_2O_9$

Zero layer				First layer			
00l	I'₁	I <sub>obs.</sub>	I'₂	21l	I'₁	I <sub>obs.</sub>	I'₂
4	11	m-	32	1	1.7	—	14
6	1.4	vvw	1.4	3	18	vw	4.8
8	28	m-	14	5	330	st	340
10	360	vst	360	7	18	—	0.4
12	45	w	11	9	23	w	67
14	50	m <sup>+</sup>	88	11	4.8	—	3.6
16	6.3	vw	5.8	13	26	vw	28
18	70	m	38	15	300	w	280
20	280	st	230	17	18	—	0.3
22	25	—	0.4	19	42	w <sup>+</sup>	150
24	58	m <sup>+</sup>	250	21	14	—	7.8
26	21	w-	10	23	66	w <sup>+</sup>	36
28	85	m-	21	25	210	m	170
30	240	m	120	27	23	—	2.9
32	17	w	6.8				
10l	I'₁	I <sub>obs.</sub>	I'₂	11l	I'₁	I <sub>obs.</sub>	I'₂
1	1.0	m-	8.4	2	18	vw	1.2
3	14	m-	4.0	4	9.0	m	34
5	320	vst	340	6	0.1	m	8.4
7	16	—	0.5	8	25	w	14
9	24	m	67	10	350	m <sup>+</sup>	340
11	6.3	—	2.0	12	19	—	0.2
13	24	w	24	14	36	vw	100
15	310	st	280	16	9.6	—	4.8
17	13	—	0.5	18	45	w	31
19	42	m <sup>+</sup>	160	20	280	m <sup>+</sup>	230
21	14	vw	7.8	22	22	—	0.0
23	64	m	38	24	71	m	200
25	210	m	170	26	27	vw	14
27	23	—	2.9	28	85	w	26
29	81	m <sup>+</sup>	220	30	190	m	130
31	32	w	24				
20l	I'₁	I <sub>obs.</sub>	I'₂				
2	12	vw	1.4				
4	10	w	36				
6	0.5	—	4.8				
8	31	w-	14				
10	350	m	350				
12	41	—	7.8				
14	50	w	88				
16	6.3	—	6.8				
18	69	w	40				
20	280	m <sup>+</sup>	230				
22	25	—	0.4				
24	59	m <sup>+</sup>	240				
26	20	vw	11				
28	85	w	21				

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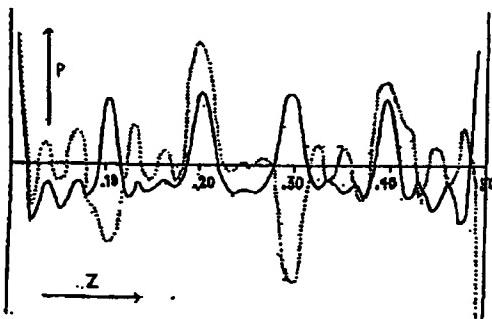
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## ARKIV FÖR KEMI. Bd 1 nr 54

Figure 1a. Patterson function of  $\text{Pb}_2\text{Bi}_2\text{Nb}_2\text{O}$ , along  $00z$ 

$$\text{Full curve: } \sum_l I_{00l} \cos 2\pi lz$$

$$\text{Dotted curve: } \sum_l I_{11l} \cos 2\pi lz \text{ (orthorhombic indices).}$$

Figure 1b. Patterson function of  $\text{Bi}_2\text{NbTiO}$ , along  $00z$ 

Of 8-fold positions only  $\pm 00z$  is possible.

It was assumed arbitrarily that 4 Me occupy the position  $000$ .

Using the distances found with the aid of the Patterson function, two possibilities for placing the Nb atoms arose:

- |                          |               |                       |
|--------------------------|---------------|-----------------------|
| 1. 8 Nb in $\pm 00 0.20$ | 4 Me in $000$ | 8 Me in $\pm 00 0.40$ |
| 2. 8 Nb in $\pm 00 0.40$ | 4 Me in $000$ | 8 Me in $\pm 00 0.20$ |

The two curves on the graph were added and the areas under the peaks at 0.20 and 0.40 calculated. The ratio 1.5:1 was found for 0.20/0.40.

In case 1, the ratio was calculated to be 0.91:1 and in case 2, 1.1:1 if the ratio  $f_{\text{Nb}}/f_{\text{Me}}$  was assumed to be 0.46. These figures cannot be compared directly with the observed ratio 1.5:1 since the zero level in figure 1 is of course uncertain. Case 2 agrees slightly better insofar as the peak at 0.20 is actually higher. It seemed, however, that the uncertainty in determining the areas was so large that case 1 could not be excluded by these measurements alone.

B. AURIVILLIUS, *Mixed bismuth oxides with layer lattices*

## Case 1

In calculating the structure amplitudes  $z_{Nb}$  was varied around 0.20 and  $z_{Me}$  around 0.40. The average ratio  $f_{Nb}/f_{Me}$  was assumed to be 0.46. The intensities were compared with calculated values of  $A^2$ :

$A = 10 (\cos 2\pi l z_{Me} + 0.46 \cos 2\pi l z_{Nb} + 0.5) = 10 F/4 f_{Me}$ . In this way the best values for the parameters were found to be:

$z_{Me} = 0.397 \pm 0.002$  and  $z_{Nb} = 0.192 \pm 0.004$ . In Table 1a  $I_{calo}$  is compared with the observed intensities.

## Case 2

$z_{Nb}$  was varied about 0.40 and  $z_{Me}$  around 0.20. The best values were found to be  $z_{Nb} = 0.412 \pm 0.004$  and  $z_{Me} = 0.202 \pm 0.002$ .

The observed and calculated values are compared in Table 1a.

It was found that arrangement 2 accounted slightly better for the experimental data than 1. It must, however, be borne in mind that the intensity ratios of weak spots might be changed through the influence of the oxygen atoms and that this influence was neglected in the calculations. The differences did not seem to be as large as to allow a decision between 1 and 2. It was therefore tried to find possible oxygen positions both for 1 and 2. The results were then compared.

## Case 1. Positions of the oxygen atoms

The positions of the metal atoms were assumed to be: (0 0 0;  $0 \frac{1}{2} \frac{1}{2}; \frac{1}{2} \frac{1}{2} \frac{1}{2}$ ;  $\frac{1}{2} \frac{1}{2} 0$ ) + 0 0 0 (4  $Me_1$ )  $\pm$  0 0 0.397 (8  $Me_2$ )  $\pm$  0 0 0.192 (8 Nb). Since all point positions of  $D_{2h}^{2g}$  can be described by positions of  $D_2^7$  or  $C_{2h}^{1g} a$ , only  $D_2^7$  and  $C_{2h}^{1g} a$  have been considered.

At first only  $D_2^7$  will be discussed. If the interatomic distances O-O, Me-O and Nb-O should not be smaller than 2.5, 2.2 and 1.8 Å. oxygen atoms could only be situated in the following positions:

4(b) 0 0 $\frac{1}{2}$	4(c) $\frac{1}{2} \frac{1}{2} \frac{1}{2}$	4(d) $\frac{1}{2} \frac{1}{2} \frac{1}{2}$	8(g) $\pm 0.0z$
8(h) $\frac{1}{2} \frac{1}{2} z$ ; $\frac{1}{2} \frac{1}{2} \frac{1}{2} - z$			$0.086 \leq z \leq 0.122$
		$0.039 \leq  z  \leq 0.061$	$0.262 \leq z \leq 0.311$
		$0.148 \leq  z  \leq 0.201$	
8(i) $\frac{1}{2} y \frac{1}{2}$ ; $\frac{1}{2} \frac{1}{2} - y \frac{1}{2}$	8(j) $x \frac{1}{2} \frac{1}{2}$ ; $\frac{1}{2} - x \frac{1}{2} \frac{1}{2}$		
$y = 0$		$x = 0$	

An attempt was made to find positions for the oxygen atoms giving approximately regular octahedra around Nb, since from known structures containing  $Nb^{5+}$  and  $O^{2-}$  this seemed to be the normal configuration  $Nb^{5+} - O^{2-}$ . The maximum distance of contact Nb-O was assumed to be 2.5 Å.

With these assumptions 8(g) and 8(h) are the only positions where oxygen atoms in contact with Nb can be situated.

With oxygen atoms in three 8-fold positions 8(h) the distances O-O would be too short. It then only remains to consider the case of oxygen atoms in two 8-fold positions 8(g) and two 8 fold positions 8(h). For the oxygen

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atoms in contact with Nb, reasonable interatomic distances were obtained assuming: 8 O<sub>2</sub> in 8(g)  $z_2 = 0.100$  8 O<sub>3</sub> in 8(g)  $z_3 = 0.264$  8 O<sub>4</sub> in 8(h)  $z_4 = 0.168$  8 O<sub>5</sub> in 8(h)  $z_5 = -0.168$ . Even if small adjustments of these parameters are admitted for the remaining 4 O there is room only in the position 00 $\frac{1}{2}$  (O<sub>1</sub>). With these assumptions the distances would be:

$$\begin{array}{lll} \text{Me}_1-4 \text{ O}_1 = 2.75 & \text{Me}_2-4 \text{ O}_2 = 2.75 & \text{Nb}-\text{O}_2 = 2.34 \\ \text{Me}_1-2 \text{ O}_3 = 2.55 & \text{Me}_2-2 \text{ O}_4 = 2.55 & \text{Nb}-2 \text{ O}_4 = 2.04 \\ & \text{Me}_2-2 \text{ O}_5 = 2.55 & \text{Nb}-\text{O}_5 = 2.04 \\ \text{O}_4-4 \text{ O}_5 = 2.74 & & \text{Nb}-\text{O}_3 = 1.84 \\ \text{O}_3-2 \text{ O}_4 = 2.60 & & \\ \text{O}_3-2 \text{ O}_5 = 2.60 & & \\ \text{O}_1-2 \text{ O}_2 = 2.55 & & \end{array}$$

It is seen that the positions given might equally well be described by  $D_{2h}^{23}$  or if the pseudo-tetragonal unit cell ( $a = 3.89$   $c = 25.53$  Å) is chosen by  $D_{2h}^{17}$ .

As  $a \sim b$  and the positions of the oxygen atoms must be chosen from space considerations, the discussion will be the same for  $C_{2h}^{18}$  as for  $C_{2v}^{18}$ . For  $C_{2v}^{18}$  it is found that the oxygen atoms can be only in the planes  $y = 0$   $y = 0.25 \pm 0.03$   $y = \frac{1}{2}$  and  $y = 0.75 \pm 0.03$ . For  $y = 0$  or  $\frac{1}{2}$ ,  $z$  must either be 0 or  $\frac{1}{2}$  or lie between the limits  $0.049 < |z| < 0.451$ , otherwise the distance O-O will be  $< 2.5$  Å. For  $y = \frac{1}{2}$  or  $\frac{3}{2}$ ,  $z$  must have the values 0,  $\frac{1}{2}$ ,  $\frac{1}{2}$  or  $\frac{3}{2}$  or lie between the limits  $0.049 < |z| < 0.201$   $0.299 < |z| < 0.451$ .

In figure 2a sections of the unit cell are made for  $y = 0$  and  $y = \frac{1}{2}$ . Possible regions with space group  $C_{2v}^{18}$  are denoted in the figure by shaded areas. For these areas the distances  $O-O \geq 2.5$  Å,  $\text{Me}-O \geq 2.2$  and  $\text{Nb}-O \geq 1.8$  Å.

With space group  $C_{2v}^{18}$  it thus seems that no basically new atomic positions are obtained, although this symmetry allows the atoms to be slightly shifted from the positions of  $D_2^T$ .

In Table 1 the intensities have been calculated from the parameters found and compared with the observed ones. (The calc. intensities are denoted by  $I_1$ ). The mode of calculation is shown by the calculation of  $I_{001}$ .  $I = A^2$ .

$A = 10 (0.5 + \cos 2\pi l z_{\text{Me}} + (f_{\text{Nb}}/f_{\text{Me}}) \cos 2\pi l z_{\text{Nb}} + (f_0/f_{\text{Me}}) (0.5 + \cos 2\pi l z_2 + \cos 2\pi l z_3 + 2 \cos 2\pi l z_4))$ . Since the ratios  $f_{\text{Nb}}/f_{\text{Me}}$  and  $f_0/f_{\text{Me}}$  vary with  $\sin \theta/\lambda$  they were interpolated from values given in the International Tables (1).

### Case 2. Positions of the oxygen atoms

The positions of the metal atoms were assumed to be:  $(000; \frac{1}{2} \frac{1}{2} 0; 0 \frac{1}{2} \frac{1}{2}; \frac{1}{2} 0 \frac{1}{2}) + 000$  (4 Me<sub>1</sub>)  $\pm 000$  0.202 (8 Me<sub>2</sub>)  $\pm 000$  0.412 (8 Nb).

With  $D_2^T$  the following positions are available for the oxygen atoms 4(b) 00 $\frac{1}{2}$

8(g) $\pm 00z$	8(h) $\frac{1}{2} \frac{1}{2} z, \frac{1}{2} \frac{1}{2} \frac{1}{2} - z$
$0.086 \leq z \leq 0.116$	$0.039 \leq  z  \leq 0.161$
$0.288 \leq z \leq 0.342$	
4(c) $\frac{1}{2} \frac{1}{2} \frac{1}{2}$	4(d) $\frac{1}{2} \frac{1}{2} \frac{3}{4}$
16(k) $xyz, \bar{x}\bar{y}z, x\bar{y}\bar{z}, \bar{x}y\bar{z}$	
$x = 0$	$x = 0.25 \pm 0.03$
$y = 0.25 \pm 0.03$ or $y = 0$	
$z \sim 0.135$	

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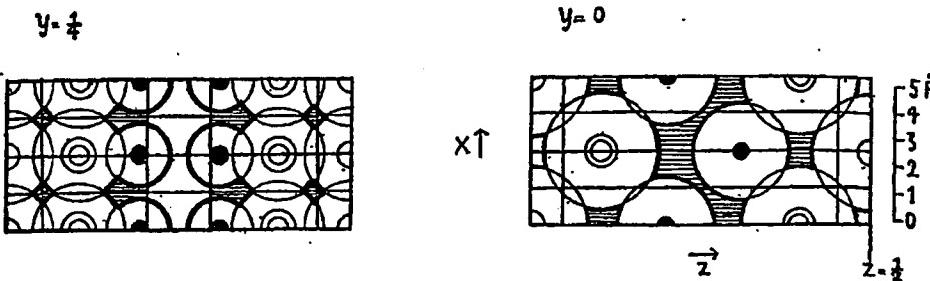


Figure 2 a (see Case 1 in the text.)

The projection of the positions of the Nb,  $\text{Me}_1$  and  $\text{Me}_2$  atoms on the planes  $y = 0$  and  $y = \frac{1}{4}$  are denoted by: black circles, white circles and double circles respectively.

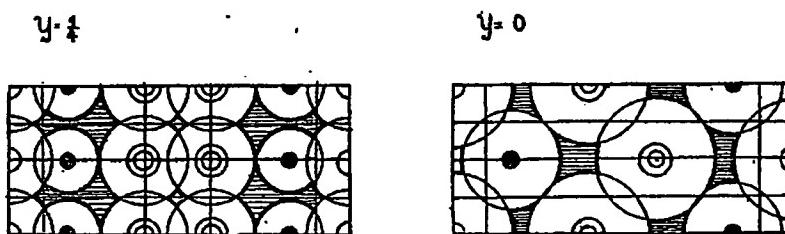


Figure 2 b (see Case 2 in the text.)

It was found that oxygen atoms in the positions 4(c), 4(d) or 16(k) could not be part of an octahedron around Nb. With O in the remaining positions 4(b), 8(g) and 8(h), octahedra around Nb might be achieved in the following ways:  $(1.8 \leq \text{Nb}-\text{O} \leq 2.5)$ .

With oxygen atoms in three 8-fold positions 8(h), it seemed impossible to find positions for the remaining 12 oxygen atoms giving O-O distances  $\leq 2.5 \text{ \AA}$ .

With two 8-fold positions 8(h) + 4(b) + one 8-fold position 8(g) the following positions were assumed for oxygen atoms in contact with Nb:

$$\begin{array}{lll} 4 \text{ O}_1 \text{ in } 4(\text{b}) & 8 \text{ O}_3 \text{ in } 8(\text{g}) & z = 0.324 \\ 8 \text{ O}_3 \text{ in } 8(\text{h}) & z = 0.088 & 8 \text{ O}_4 \text{ in } 8(\text{h}) \quad z = -0.088. \end{array}$$

For the remaining 8 oxygen atoms there was only room in the positions 4(c) and 4(d). ( $\text{O}_5, \text{O}_6$ ).

With the above assumptions the distances would be:

$$\begin{array}{lll} \text{Me}_1-4 \text{ O}_1 = 2.75 & \text{Me}_2-2 \text{ O}_5 = 2.29 & \text{Nb}-\text{O}_1 = 2.24 \\ \text{Me}_1-4 \text{ O}_3 = 2.96 & \text{Me}_2-2 \text{ O}_6 = 2.29 & \text{Nb}-2 \text{ O}_3 = 1.94 \\ \text{Me}_1-4 \text{ O}_4 = 2.96 & \text{Me}_2-4 \text{ O}_2 = 2.82 & \text{Nb}-2 \text{ O}_4 = 1.94 \\ & & \text{Nb}-\text{O}_2 = 2.24 \\ \text{O}_5-4 \text{ O}_6 = 2.75 & \text{O}_2-2 \text{ O}_6 = 2.70 & \text{O}_2-2 \text{ O}_3 = 2.96 \\ \text{O}_3-4 \text{ O}_4 = 2.75 & \text{O}_2-2 \text{ O}_5 = 2.70 & \text{O}_3-2 \text{ O}_4 = 2.96 \\ \text{O}_1-4 \text{ O}_3 = 2.96 & \text{O}_1-4 \text{ O}_4 = 2.96 & \end{array}$$

The above positions might be equally well described by  $D_{2h}^{28}$  or if a pseudo-tetragonal unit cell is assumed ( $a = 3.89 \text{ \AA}, c = 25.53$ ) by  $D_{4h}^{16}$ .

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In Figure 2 b sections are made of the unit cell for  $y = 0$  and  $y = \frac{1}{4}$  showing the positions possible for the oxygen atoms if the space group  $C_{2h}^{18}a$  is assumed. Possible regions are denoted by shaded areas. It was found that only with oxygen atoms situated near the positions given above, could octahedra of O around all Nb atoms and reasonable distances to O be attained.

Thus no new arrangements were found when space group  $C_{2h}^{18}a$  was assumed. In Table 1 the intensities are calculated from the parameters given above. The calculated intensities are denoted by  $I_2'$ . The mode of calculation is the same as was used in case 1. It is seen from the Table that both 1 and 2, in which cases the influence of the oxygen atoms was neglected, account fairly well for the experimental data. From this follows that the calculated intensities  $I_1$  and  $I_2'$ , where regard was taken to the O atoms, do not differ much either. Although the ratio 211:213 (see Table 1 (pseudo-tetragonal indices)) is best described by 1', 2' on the whole seemed to satisfy the observed intensities best (see for instance the intensity ratios 112:114 116:118 202:204 101:103 and 107:109). No definite conclusions could however be drawn from the study of  $PbBi_2NbO_9$  alone.

 $Bi_3NbTiO_9$ 

Just as for  $PbBi_2Nb_2O_9$ , there was nothing in the Weissenberg photographs to indicate a lower Laue symmetry than  $D_{4h}-4/mmm$ . From the powder photographs (Table 6 a) it is however seen that the actual unit cell is orthorhombic with axes  $a = 5.405$   $b = 5.442$   $c = 25.11 \text{ \AA}$ .

The intensities of the spots in the Weissenberg photographs indicate that the metal atoms are probably placed on the lines  $00z$ . The Patterson function (Fig. 1 b) showed high maxima at 0.20 and 0.40. If the same assumptions are made as for  $PbBi_2Nb_2O_9$  the following arrangements seemed to be possible:

A. 4 Nb in $000$	B. 4 Ti in $000$	$C_1$ 4 Bi in $000$
8 BiTi in $\pm 00z_1$	8 BiNb in $\pm 00z_1$	8 NbTi in $\pm 00z_1$
8 BiTi in $\pm 00z_2$	8 BiNb in $\pm 00z_2$	8 Bi in $\pm 00z_2$
$C_2$ 4 Bi in $000$		
8 NbTi in $\pm 00z_2$	$z_1 \sim 0.20$	$z_2 \sim 0.40$
8 Bi in $\pm 00z_1$		

The areas under the peaks at 0.20 and 0.40 were calculated as for  $PbBi_2Nb_2O_9$  and the ratio 0.20/0.40 was found to be 1.4. The calculated ratios for A, B,  $C_1$  and  $C_2$  were 1.0, 1.0, 0.84 and 1.2. The area ratio for  $C_2$  agreed best with the observed one. The differences are however small, so that all alternatives were considered. The intensities were calculated as for  $PbBi_2Nb_2O_9$ . The ratios  $f_{Ti}/f_{BiNb}$ ,  $f_{Nb}/f_{BiTi}$  and  $f_{NbTi}/f_{Bi}$  were assumed to be 0.26, 0.57 and 0.34. The calculated and observed intensities for A and B are compared in Table 2. In these calculations the influence of the oxygen atoms was neglected. The best agreement was found for

	$z_1$	$z_2$
A	0.198	0.400
B	0.196	0.400

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Table 2  
Weissenberg photographs of  $\text{Bi}_3\text{NbTiO}_8$ .

$l$	$I_A$	$I_B$	$I_{00l}$	$\frac{I_{obs.}}{I_{11l}}$	$I_{20l}$
2	4.0	12	—	vw	vw
4	7.3	22	m	st	$m^+$
6	2.3	5.3	w	st	m
8	7.3	22	m	w	m
10	510	440	st	st	st
12	1.4	2.6	w	—	vw
14	15	52	$m^+$	vw	w
16	0.2	0.0	w	vw	—
18	11	30	$m^+$	w	vw
20	500	400	st	st	$m^+$
22	0.1	0.4	—	—	—
24	27	94	m	m	m
26	0.5	2.0	w	m	m
28	14	31	m	$m^+$	$m^+$
30	490	350	m	$m^+$	—
$l$	$I_A$	$I_B$	$I_{10l}$	$I_{21l}$	
1	4.4	12	st	$m^+$	
3	5.8	17	m	vw	
5	520	450	vst	vst	
7	2.6	6.3	—	—	
9	11	35	m	m	
11	0.8	1.4	w	w	
13	9.0	27	vw	w	
15	510	420	st	w	
17	0.6	0.3	—	—	
19	20	70	w	w	
21	0.0	0.5	w	w	
23	12	31	m	m	
25	500	380	$m^+$	$m^+$	
27	0.0	3.2	—	—	
29	34	120	m		
31	1.4	4.4	m		

One half  
notes the

The f  
8 NbTi  
following

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4 Bi i  
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4 O<sub>1</sub> in

From Table 2 it is seen that A and B account quite well for the observed intensities.

With A and B, Bi and Ti or Bi and Nb would occupy the same point position. This seemed *a priori* unlikely and if it was assumed that  $\text{Bi}_3\text{NbTiO}_8$  and  $\text{PbBi}_3\text{Nb}_2\text{O}_9$  were built up in the same way, arrangements A and B would imply that Pb, Bi and Nb were distributed over one point position, in  $\text{PbBi}_3\text{Nb}_2\text{O}_9$ . Therefore, although arrangements A and B cannot be excluded from intensity discussions alone, they seem very improbable and will not be dealt with in the following.

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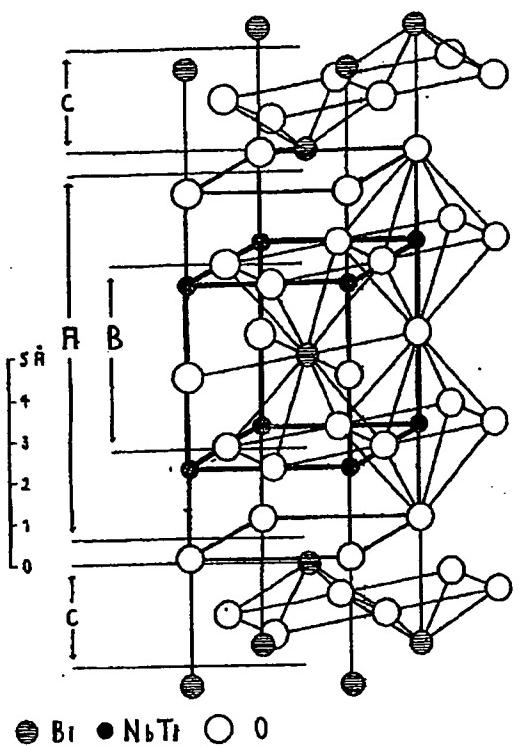


Figure 3.

One half of the pseudo-tetragonal unit cell of  $\text{Bi}_3\text{NbTiO}_9$  (from  $z=0.25$  to  $z=0.75$ ). A denotes the perovskitic layer  $\text{BiNbTiO}_6^+$ , C  $\text{Bi}_2\text{O}_3$  layers and B the unit cell of a hypothetical perovskite structure  $\text{BiNb}_{0.5}\text{Ti}_{0.5}\text{O}_6$ .

### Case C<sub>1</sub>

The following positions were assumed: 4 Bi in 000, 8 Bi in  $\pm 00 0.396$ , 8 NbTi in  $\pm 00 0.192$ . By the same arguments as used for  $\text{PbBi}_2\text{Nb}_2\text{O}_9$ , the following positions were arrived at:

$$\begin{array}{lll} 4 \text{ O}_1 \text{ in } 00\frac{1}{2} & 8 \text{ O}_2 \text{ in } \pm 00 0.092 & 8 \text{ O}_3 \text{ in } \pm 00 0.268 \\ 8 \text{ O}_4 \text{ in } \frac{1}{2}\frac{1}{2}z; \frac{1}{2}\frac{1}{2}\frac{1}{2}-z & z = 0.164 \\ 8 \text{ O}_5 \text{ in } \frac{1}{2}\frac{1}{2}z; \frac{1}{2}\frac{1}{2}\frac{1}{2}-z & z = -0.164. \end{array}$$

In Table 3 the intensities are calculated from these parameters.

### Case C<sub>2</sub>

4 Bi in 000, 8 Bi in  $\pm 00 0.200$  and 8 NbTi in  $\pm 00 0.412$  were assumed. In case 2' (see  $\text{PbBi}_2\text{Nb}_2\text{O}_9$ ) the parameters for the oxygen atoms would be 4 O<sub>1</sub> in 00 $\frac{1}{2}$ , 8 O<sub>2</sub> in  $\pm 00 0.324$ , 4 O<sub>5</sub> in  $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ,

$$\begin{array}{lll} 4 \text{ O}_6 \text{ in } \frac{1}{2}\frac{1}{2}\frac{1}{2}, 8 \text{ O}_4 \text{ in } \frac{1}{2}\frac{1}{2}z; \frac{1}{2}\frac{1}{2}\frac{1}{2}-z & z = 0.088 \\ 8 \text{ O}_3 \text{ in } \frac{1}{2}\frac{1}{2}z; \frac{1}{2}\frac{1}{2}\frac{1}{2}-z & z = -0.088 \end{array}$$

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Table 3  
Weissenberg photographs of  $\text{Bi}_3\text{NbTiO}_9$

Zero layer				First layer			
00l	$I_{C'_1}$	$I_{\text{obs.}}$	$I_{C'_3}$	21l	$I_{C'_1}$	$I_{\text{obs.}}$	$I_{C'_3}$
4	13	m	36	1	2.6	m+	22
6	0.5	w	10	3	35	vw	6.3
8	48	m	16	5	290	vst	300
10	310	st	330	7	19	—	1.0
12	48	w	12	9	27	m	55
14	38	m+	59	11	3.6	w	18
16	2.6	w	29	13	52	w	26
18	100	m+	48	15	270	w	270
20	240	st	240	17	6.8	—	0.8
22	12	—	0.5	19	45	w	90
24	42	m	140	21	14	w	40
26	29	w	42	23	110	m	46
28	100	m	35	25	200	m+	200
30	190	m	160				
10l	$I_{C'_1}$	$I_{\text{obs.}}$	$I_{C'_3}$	11l	$I_{C'_1}$	$I_{\text{obs.}}$	$I_{C'_3}$
1	2.0	st	17	2	34	vvw	2.6
3	29	m	5.3	4	2.9	st	41
5	270	vst	300	6	6.8	st	68
7	17	—	1.2	8	62	w	22
9	29	m	56	10	360	st	310
11	5.8	w	15	12	14	—	1.0
13	49	vw	28	14	29	vw	76
15	270	st	270	16	10	vw	40
17	5.3	—	0.6	18	64	w	16
19	44	w	92	20	250	st	210
21	16	w	38	22	21	—	0.0
23	110	m	46	24	66	m	92
25	200	m+	200	26	32	m	61
27	4.4	—	1.2	28	130	m+	27
29	65	m	110	30	150	m+	200
31	41	m	76				
20l	$I_{C'_1}$	$I_{\text{obs.}}$	$I_{C'_3}$				
2	18	vw	2.9				
4	12	m+	87				
6	0.1	m	16				
8	48	m	17				
10	300	st	320				
12	33	vw	5.8				
14	37	w	58				
16	2.6	—	31				
18	100	vw	45				
20	240	m+	240				
22	12	—	0.5				
24	42	m	140				
26	29	m	45				
28	100	m+	35				

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In Table 3 the intensities are calculated with these assumptions.. It is seen from the Table that with  $C_1$  the order of the reflections 101:103, 211:213, 002:204 and 107:109 are reversed. The same result was obtained if the influence of the oxygen atoms was neglected. If  $\epsilon_{Bi}$  and  $\epsilon_{NbTi}$  were varied around 0.396 and 0.192 so as to give correct ratios for some of these reflections, large discrepancies occurred for other reflections. With  $C_2$  the intensities turned out to be of the right order. There are however a few discrepancies. 00 20 is certainly stronger than 0018 and  $00\bar{3}0 > 0028$ , but the calculated ratios seem to be too large. On the whole the agreement is however good.

Thus if the X ray data for only one of  $PbBi_2Nb_2O_9$  or  $Bi_3NbTiO_9$  were considered, different atomic arrangements appeared to be possible, whereas only seems to explain the observed data both for  $PbBi_2Nb_2O_9$  and  $Bi_3NbTiO_9$ .

With orthorhombic description the positions will be:

$D_{2h}^{23} - mmm$

(000; $0\frac{1}{2}\frac{1}{2}$ ; $\frac{1}{2}0\frac{1}{2}$ ; $\frac{1}{2}\frac{1}{2}0$ ) +
4 $Bi_1$ ( $Me_1$ ) in 4 (a) 000
8 $Bi_2$ ( $Me_2$ ) in 8 (i) $\pm 00 0.200$ (0.202)
8 $NbTi$ (Nb) in 8 (i) $\pm 00 0.412$ (0.412)
4 $O_1$ in 4 (b) $00\frac{1}{2}$
8 $O_2$ in 8 (i) $00 0.324$ (0.324)
8 $O_3$ in 8 (f) $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ; $\frac{1}{2}\frac{1}{2}\frac{1}{2}$
16 $O_4$ in 16 (j) $\frac{1}{2}\frac{1}{2}z$ ; $\frac{1}{2}\frac{1}{2}\bar{z}$ ; $\frac{1}{2}\frac{1}{2}z$ ; $\frac{1}{2}\frac{1}{2}\bar{z}$
$z = 0.088$ .

With pseudo-tetragonal description the positions will be:

$D_{4h}^{17} - I 4/mmm$

(000; $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ) +
2 $Bi_1$ ( $Me_1$ ) in 2 (a) 000
4 $Bi_2$ ( $Me_2$ ) in 4 (e) $\pm 00 0.200$ (0.202)
4 $NbTi$ (Nb) in 4 (e) $\pm 00 0.412$ (0.412)
2 $O_1$ in 2 (b) $00\frac{1}{2}$
4 $O_2$ in 4 (e) $\pm 00 0.324$ (0.324)
4 $O_3$ in 4 (d) $0\frac{1}{2}\frac{1}{2}$ ; $\frac{1}{2}0\frac{1}{2}$
8 $O_4$ in 8 (g) $\pm (0\frac{1}{2}z; \frac{1}{2}0z)$ $z = 0.088$ .

Table 4

Values of the tolerance factor,  $t$ , for different compounds having the  $CaBi_2Nb_2O_9$  structure.

Compound	$t. 100$
$Bi_3NbTiO_9$	91
$Bi_3TaTiO_9$	91
$CaBi_2Nb_2O_9$	91
$SrBi_2Nb_2O_9$	99
$SrBi_3Ta_2O_9$	99
$BaBi_2Nb_2O_9$	106
$PbBi_2Nb_2O_9$	101
$NaBi_2Nb_2O_{18}$	91
$KBi_2Nb_2O_{18}$	97

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Table 5 (co

Powder photographs of  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  and  $\text{SrBi}_2\text{Nb}_2\text{O}_9$ . Cr K radiation. Pseudo tetragonal indices.

 $\text{CaBi}_2\text{Nb}_2\text{O}_9$ 

$h k l$	$I_{\text{obs.}}$	$I_\alpha$	$I_\beta$	$I_\gamma$
0 0 6	—	8.4	0.8	0.01
0 0 8	m	61	9.6	0.6
1 1 4 + 0 0 1 0	(m)	230	230	230
0 0 1 2	—	0.5	19	47
0 0 1 4	vw	29	46	56
0 0 1 6	vw	2.6	0.6	4.0
0 0 1 8	w	100	34	13
1 0 1	—	1.2	0.5	2.9
1 0 3	st	36	1.4	1.4
1 0 5	vst	200	200	200
1 0 7	w	21	0.3	7.8
1 0 9	vvw	18	32	43
1 0 1 1	—	7.0	0.2	0.5
1 0 1 3	m+	79	19	4.4
2 0 1 0 + 1 0 1 5	(st)	160	160	160
2 1 1 1 + 1 0 1 7	(w)	22	0.2	9.0
1 1 2	—	26	0.04	4.8
0 0 1 0 + 1 1 4	(m)	4.4	14	22
1 1 6	w	4.4	17	28
1 1 8	m	69	13	1.7
2 0 4 + 1 1 1 0	(st)	200	200	200
1 1 1 2	—	22	0.1	8.4
1 1 1 4	w	41	61	72
2 0 2	w	27	0.1	4.4
1 1 1 0 + 2 0 4	(st)	3.6	13	20
2 0 6	w	3.2	0.04	1.4
2 1 5 + 2 0 8	(st)	59	9.0	0.5
1 0 1 5 + 2 0 1 0	(st)	220	220	220
2 0 1 2	vw	1.4	15	41
2 1 1	w	0.1	2.3	6.3
2 1 3	w	38	2.0	1.0
2 0 8 + 2 1 5	(st)	210	210	210
2 1 7	—	21	0.3	7.8
2 1 9	vvw	18	33	43
1 0 1 7 + 2 1 1 1	(w)	4.4	0.01	1.4
One half tioned in determine 0 0 0.202. Ca, Sr, Ba $\text{KBi}_5\text{Nb}_4\text{O}_{11}$ do not diff valid for tL Ca, Sr, Ba				
$\alpha$ Only 1 $\beta$ Random $\gamma$ Only 1				
$\text{SrBi}_2\text{Nb}_2\text{O}_9$				
0 0 6	—	3.2	0.1	0.2
0 0 8	vw	46	11	2.6
1 1 4 + 0 0 1 0	(m)	260	260	260
0 0 1 2	vw	0.2	16	35
0 0 1 4	m	42	58	64
0 0 1 6	—	0.3	1.4	4.4
0 0 1 8	w	83	35	18
0 0 2 0	st	160	160	160

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Table 5 (cont.)

Pseudo

	<i>hkl</i>	<i>I<sub>obs.</sub></i>	<i>I<sub>a</sub></i>	<i>I<sub>β</sub></i>	<i>I<sub>γ</sub></i>
	1 0 1	—	0.0	2.0	4.0
	1 0 3	vw	24	2.0	0.1
	1 0 5	st	230	240	230
	1 0 7	—	12	0.01	3.6
	1 0 9	w	28	42	49
	1 0 11	—	2.3	0.01	0.8
01	1 0 13	m	61	20	8.4
6	2 0 10+1 0 15	(st)	190	200	200
—	$\beta$ 0 0 2 0+2 2 0+1 0 1 7	(m)	13	0.01	4.0
	1 0 19	m	88	110	120
0	1 1 2	—	16	0.3	1.7
	0 0 1 0+1 1 4	(m)	10	20	26
	1 1 6	vw	10	22	29
	1 1 8	w	52	14	4.4
	1 1 1 0	st	230	240	230
	1 1 1 2	—	13	0.0	3.6
	1 1 1 4	w	56	74	81
	1 1 1 6	—	0.1	4.0	8.4
	1 1 1 8	m	40	10	2.3
	2 0 2	—	17	0.4	1.4
	2 0 4	—	9.0	19	24
	2 0 6	—	0.5	0.8	2.3
	$\beta$ 1 1 1 4+2 0 8	(w)	43	10	2.3
	1 0 1 5+2 0 1 0	(st)	250	260	250
	$\beta$ 2 1 1 3+2 0 1 2	(vw)	0.01	12	29
	2 0 1 4	w	42	58	64
	2 0 1 6	—	0.2	1.7	4.8
	2 1 1	w	0.6	4.8	7.8
	2 1 3	w	26	2.6	0.01
	2 1 5	st	240	240	240
	2 1 7	—	12	0.01	3.6
	2 1 9	vw	27	42	49
	2 1 1 1	—	1.2	0.4	2.0
	2 1 1 3	m	59	19	7.8
	2 0 1 0+2 1 1 5	(st)	190	190	190

One half of the pseudo-tetragonal unit cell is pictured in figure 3. As mentioned in the discussion on  $PbBi_2Nb_2O_9$ , it was impossible in this phase to determine how Pb and Bi are distributed over the point positions 0 0 0 and 0 0 0.202. It therefore seemed of interest to try to determine the positions of 0 0 0.202. It therefore seemed of interest to try to determine the positions of Ca, Sr, Ba and K in the compounds  $CaBi_2Nb_2O_9$ ,  $SrBi_2Nb_2O_9$ ,  $BaBi_2Nb_2O_9$  and  $KBi_2Nb_2O_9$ . As the cell dimensions of the Pb, Ca, Sr, Ba and K compounds do not differ much it was assumed that the parameters of  $PbBi_2Nb_2O_9$  are also valid for the other compounds. There were three extreme ways of distributing Ca, Sr, Ba and K over the positions 0 0 0 and 0 0 0.202:

$\alpha$  Only Bi in 0 0 202

$\beta$  Random distribution

$\gamma$  Only Bi in 0 0 0.

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*Table 6 a*  
Powder photographs of  $\text{Bi}_2\text{NbTiO}_9$ . Cr K radiation.

Orthorhombic indices.

$h k l$	$10^4 \sin^2 \theta_{\text{calc.}}$	$10^4 \sin^2 \theta_{\text{obs.}}$	$I_{\text{obs.}}$	$h k l$	$10^4 \sin^2 \theta_{\text{calc.}}$	$10^4 \sin^2 \theta_{\text{obs.}}$	$I_{\text{obs.}}$	$h k l$	$I_{\text{obs.}}$
1 1 1	0914	0909	m	0 2 1 4	5856	5874	m	1 0 1	
1 1 3	1080	1072	w+	2 0 1 4	5878	5990	vw	1 0 3	
0 0 8	1333	1319	w+	—	—	6128	w+	0 0 8	
1 1 5	1414	1413	vst	1 3 9	6128	6172	w+	1 0 5	
0 2 0	1774	1767	m+	3 1 9	6172	6175	w+	1 1 0	
2 0 0	1796	1790	m	—	—	6250	vvw	0 0 1 0	
0 0 1 0	2083	2078	m	2 2 1 2	6569	6573	vvw	1 1 4	
2 0 4	2129	2131	w	0 0 1 8	6747	6747	vw	β 1 0 9	
β 1 1 9	2136	2324	vvw	1 3 1 1	6961	6961	w	1 1 6	
—	—	—	—	0 4 0	7097	7097	m	1 0 9	
0 2 6	2624	2530	m	0 2 1 6	7105	7107	m	β 2 0 0	
2 0 6	2546	2546	m	2 0 1 6	7127	7182	m	0 0 1 2	
1 1 9	2580	2585	m	0 4 2	7180	7182	m	1 1 8	
—	—	2739	vvw	4 0 0	7185	7388	w	1 0 1 1	
0 2 8	3107	3129	w	β 2 4 0	7357	7388	w	2 0 0	
2 0 8	3129	—	β 4 2 0	7420	7430	—	1 1 1 0		
1 1 1 1	3413	3415	w	0 4 4	7430	7648	w	0 0 1 4	
—	—	3523	w	2 2 1 4	7652	7836	vvw	1 0 1 3	
2 2 0	3570	3576	st	0 4 6	7847	—	2 1 1		
2 2 2	3653	3648	vw	4 0 6	7935	8005	w	2 0 8	
β 1 1 1 3	3654	—	vw	1 3 1 3	7960	—	2 1 5		
0 2 1 0	3857	3860	st	3 1 1 3	8004	—	1 0 1 5		
2 0 1 0	3879	—	st	3 3 1	8054	—	2 0 1 0		
0 0 1 4	4082	4089	w	0 0 2 0	8330	—	—	—	
β 1 3 5	4103	4236	vw	1 1 1 9	8411	8409	m	—	
—	—	4236	vw	0 4 8	8430	—	—	—	
2 2 6	4320	4324	w	2 0 1 8	8543	8558	st	—	
1 1 1 3	4412	4414	w	3 3 5	8554	—	—	—	
1 3 1	4462	4454	w	2 4 0	8887	8888	m	—	
3 1 1	4506	4504	vw	2 2 1 6	8901	—	—	—	
β 1 1 1 5	4621	4623	w	4 2 0	8969	8963	m	—	
1 3 3	4628	—	w	2 4 2	8970	—	—	—	
3 1 3	4672	4676	w	1 3 1 5	9127	9105	st	—	
β 2 2 1 0	4679	4676	w	3 1 1 5	9171	9156	vst	—	
2 2 8	4903	4896	w	0 4 1 0	9180	9189	m	—	
1 3 5	4962	4956	st	4 0 1 0	9288	9264	m	—	
3 1 5	5006	5006	st	4 2 4	9292	—	—	—	
—	—	—	—	4 2 6	9709	9712	w	—	
1 1 1 5	5579	5581	st	3 3 9	9720	—	—	—	
2 2 1 0	5653	5652	st	—	—	—	—	—	

The intensities were calculated for these possibilities by calculations similar to those for  $\text{PbBi}_2\text{Nb}_2\text{O}_9$ , and compared with the observed ones. See Table 5. It was found that in no case did  $\gamma$  explain the observed intensities. For the Sr, Ba and K compounds the observed intensities did not permit any decision between  $\alpha$  and  $\beta$ . For  $\text{CaBi}_2\text{Nb}_2\text{O}_9$ , however, only  $\alpha$  seemed to give correct intensities. It was therefore concluded that the compounds discussed have the  $\alpha$  arrangement.

The struc  
BiNbTiO<sub>7</sub>] skite struct  
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ionic radii we  
 $\text{K}^+$  1.33,  $\text{Nb}^{5+}$   
distributed ove

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Table 6b

Powder photographs of  $\text{PbBi}_2\text{Nb}_2\text{O}_9$ . Cr K radiation.

Pseudo-tetragonal indices.

$I_{\text{obs}}$	$h k l$	$10^4 \sin^2 \theta_{\text{calc}}$	$10^4 \sin^2 \theta_{\text{obs}}$	$I_{\text{obs}}$	$h k l$	$10^4 \sin^2 \theta_{\text{calc}}$	$10^4 \sin^2 \theta_{\text{obs}}$	$I_{\text{obs}}$
m	101	0889	0892	vw	11 14	5682	5699	m
vw	103	1050	1052	vvv	219	5974	5990	m
w+	008	1288	1285	vvv	00 18	6520	6529	w
w+	105	1372	1371	vst	00 20	6663	6684	vvv
w+	110	1738	1763	m	10 17	6685		
w+	00 10	2012	2019	m	11 16	6889	6924	m
w+	114	2060	2068	vvv	305	6903	6934	m
w+	0109	2089	2068	vvv	220	6950	6976	m
w	116	2462	2489	m	20 14	7419	7435	m
m	109	2499	2499	m	21 13	7744	7749	m
m	β200	2877	2881	m	301	7839	7846	vw
m	00 12	2898	2881	m	00 20	8049	8052	m
m	118	3026	3028	w	10 19	8133	8131	m+
m	10 11	3304	3300	vvv	228	8238	8268	vw
w	200	3475	3475	st	11 18	8258		
w	11 10	3750	3755	st	305	8332	8339	m+
w	00 14	3944	3948	w+	310	8688	8673	m+
w	10 13	4289	4270	w+	21 15	8872	8690	m+
w	211	4384	4355	vvv	22 10	8962	8874	st
w	208	4763	4770	vvv	314	9010	8980	m
w	215	4847	4850	st	309	9449	9450	vvv
m	10 15	5397	5418	st				
m	20 10	5487	5493	st				

The structure of  $\text{Bi}_3\text{NbTiO}_9$  is thus built up of  $\text{Bi}_2\text{O}_3^{2+}$  layers between which  $\text{BiNbTiO}_7^{2-}$  layers are inserted. The structure may be looked upon as a perovskite structure where perovskite layers are separated by  $\text{Bi}_2\text{O}_3^{2+}$  layers. This view was supported by the fact that in all cases where the above structure was observed the radii of the ions in the layers lying between the  $\text{Bi}_2\text{O}_3^{2+}$  layers would allow for the formation of a perovskite structure. If the tolerance factor  $t$  is calculated from the ionic radii of the elements constituting the layers between the  $\text{Bi}_2\text{O}_3^{2+}$  layers, it is found to lie between the limits 0.9 and 1.1 (see Table 4), the same limits within which perovskite structures are found to be stable.

† was calculated from the formula:  $1.06 (R_A + R_O) = 0.95 \sqrt{2} (R_B + R_O)$ . (See (3).)

$$A = (K + Bi)/2 \text{ Ca, Sr, Ba etc.}$$

$$B = (Nb + Ti)/2 (Ta + Ti)/2 \text{ Nb, Ta.}$$

In the calculations case  $a$  was assumed. For calculating  $t$  the following values for the ionic radii were used:  $\text{Bi}^{3+}$  1.00,  $\text{Ba}^{2+}$  1.39,  $\text{Sr}^{2+}$  1.20,  $\text{Ca}^{2+}$  1.02,  $\text{Pb}^{2+}$  1.26,  $\text{Na}^+$  0.97,  $\text{K}^+$  1.33,  $\text{Nb}^{5+}$  0.69,  $\text{Ta}^{5+}$  0.69,  $\text{Ti}^{4+}$  0.66 and  $\text{O}^{2-}$  1.36. If, for instance, 1 K + 1 Bi are distributed over one 2-fold position the radius of (K, Bi) was taken as  $(r_K + r_{Bi})/2$ .

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The structure proposed for  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  reminds one of the structure of beyerite  $\text{CaBi}_2\text{O}_3(\text{CO}_3)_2$  described by LAGERCRANTZ and SILLÉN (4). The unit cell of beyerite is body-centered tetragonal with  $a = 3.767$  and  $c = 21.690 \text{ \AA}$ . The positions of the Ca and the Bi atoms in beyerite are Ca in 0 0 0 and  $\text{Bi} \pm 0 0 0.19$  (space group  $D_{2h}^{28}$ ), as compared with  $a = 3.860$   $c = 24.87$ , Ca in 0 0 0 and Bi in  $\pm 0 0 0.20$  for  $\text{CaBi}_2\text{Nb}_2\text{O}_9$ .

The "rotating"  $\text{CO}_3^2-$  groups in beyerite correspond to octahedral sheets  $\text{Nb}_4\text{O}_7^4-$  in  $\text{CaBi}_2\text{Nb}_2\text{O}_9$ . Following the notations given by LAGERCRANTZ and SILLÉN (4) the structure described above might also be denoted by  $X_{11}$ .

## SUMMARY

A series of tetragonal or pseudo-tetragonal phases of general composition  $(\text{Bi}, \text{Me})_6\text{R}_4\text{O}_{18}$  have been investigated.

Me: Na, K, Ca, Sr, Ba, Pb.

R: Nb, Ta, Ti.

The positions of the Me and R atoms were determined from the observed intensities and the positions of the O atoms were deduced from space considerations.

The following structure is proposed:

$D_{2h}^{28}-F mmm$

$(000; 0 \frac{1}{2} \frac{1}{2}; \frac{1}{2} 0 \frac{1}{2}; \frac{1}{2} \frac{1}{2} 0) +$

4 Bi in 4 (a) 0 0 0

8 Bi in 8 (i)  $\pm 0 0 0.200$

8 NbTi in 8 (i)  $\pm 0 0 0.412$

4 O in 4 (b) 0 0  $\frac{1}{2}$

8 O in 8 (i)  $\pm 0 0 0.324$

8 O in 8 (f)  $\frac{1}{2} \frac{1}{2} \frac{1}{2}; \frac{1}{2} \frac{1}{2} \frac{1}{2}$

16 O in 16 (j)  $\frac{1}{2} \frac{1}{2} z; \frac{1}{2} \frac{1}{2} z; \frac{1}{2} \frac{1}{2} z; \frac{1}{2} \frac{1}{2} z \quad z = 0.088$

From intensity calculations it was found that Ca in  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  and Sr, Ba, and K in the corresponding compounds are probably situated in the position 0 0 0. The proposed structure is built up of  $\text{Bi}_2\text{O}_6^{2+}$  layers alternating with single perovskite layers. The resemblance to the structure of beyerite is pointed out.

I wish to thank Professor L. G. SILLÉN for valuable discussions concerning this work.

Stockholms Högskola, Institute of Inorganic and Physical Chemistry, June 1949.

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Tryckt den 31 december 1949

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**BRIEF ATTACHMENT W**

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of

Applicants: Bednorz et al.

Serial No.: 08/479,810

Filed: June 7, 1995

Date: March 1, 2005

Docket: YO987-074BZ

Group Art Unit: 1751

Examiner: M. Kopec

For: NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION

Commissioner for Patents  
P.O. Box 1450  
Alexandria, VA 22313-1450

**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT W**

## ARKIV FÖR KEMI Band 1 nr 58

Communicated 15 September 1949 by ARNE WESTGREN and ARNE TRÆLIUS

**Mixed bismuth oxides with layer lattices****II. Structure of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$** 

By BENGT AURIVILLIUS

With 5 figures in the text

By means of X ray analysis it has been found that the crystal structures of a number of bismuth oxyhalides consist of  $\text{Bi}_2\text{O}_3^{2+}$  layers alternating with layers of halogen ions (1, 2). In all these cases the symmetry was found to be tetragonal and the lengths of the  $a$  axes almost constant  $\approx 3.8 \text{ \AA}$ .

On making an X ray study of the system  $\text{Bi}_2\text{O}_3$ — $\text{TiO}_2$  a phase (of composition about 40 atomic %  $\text{TiO}_2$ ) was found, the powder photographs of which could be explained by assuming a pseudo-tetragonal cell with  $a = 3.84$  and  $c = 32.8 \text{ \AA}$ . It seemed of interest to make a closer study of this phase since the cell dimensions and composition seemed to indicate a layer lattice with  $\text{Bi}_2\text{O}_3^{2+}$  layers, but of a type hitherto uninvestigated.

**Procedure:** Weighed amounts of  $\text{Bi}_2\text{O}_3$  (puriss) and  $\text{TiO}_2$  (puriss) were mixed and heated to about  $1100^\circ \text{C}$  for some hours in a weighed platinum crucible. After cooling the crucible was weighed again and the composition calculated by assuming that the loss of weight could be ascribed to the volatility of  $\text{Bi}_2\text{O}_3$ . Powder photographs of various preparations in the system  $\text{Bi}_2\text{O}_3$ — $\text{TiO}_2$  indicated that there is a phase with a body-centered pseudo-tetragonal unit cell with  $a = 3.841$  and  $c = 32.83 \text{ \AA}$  at compositions about 40 mole %  $\text{TiO}_2$ . It was, however, impossible to get samples which were quite free from impurities so the powder photographs always contained a few extra lines.

The lines  $21l$ ,  $22l$  and  $31l$  were found to be split up. No cleavage was, however, found for the lines  $10l$ ,  $20l$  and  $30l$ . This could be explained by assuming a face-centered orthorhombic unit cell with the same  $c$  axis as the pseudo-tetragonal cell and with its  $a$  and  $b$  axes equal to the diagonals ( $a\sqrt{2}$ ) of the pseudo cell.

The orthorhombic axes will be:  $a = 5.410$   $b = 5.448$   $c = 32.84 \text{ \AA}$ . The observed density (40 mole %  $\text{TiO}_2$ ) is 7.85. If the composition is assumed to be  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  (43 mole %  $\text{TiO}_2$ ) and 4 formula units are assumed per unit cell the calculated density will be 8.04 which agrees fairly well with the observed value.

Single crystals, thin plates, were picked out and Weissenberg photographs (zero layer and first layer) were taken around the  $3.84$  axes, thus registering  $h0l$  and  $h1l$  (pseudo cell) or  $hh1$  and  $h, h + 2, l$  (orthorhombic cell).

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Though there was nothing in the Weissenberg photographs to indicate lower Laue symmetry than  $D_{4h}$  —  $4/m\ mm\ m$ , it was — as has already been mentioned — found from the powder photographs that the real symmetry was not higher than orthorhombic (Laue symmetry  $D_{2h}$  —  $m\ mm\ m$ ).

Except for the extinctions following from the face-centering ( $h\ k\ l$  occurring only for  $h, k, l$  all odd or even) no systematic extinctions were found, which is characteristic of the space groups  $C_{2h}^{16}$ ,  $D_2^7$  and  $D_{2h}^{29}$ .

## Positions of the bismuth atoms

Since the intensities of  $h\ k\ l$  with  $h, k, l$  all odd on one side and the intensities of  $h\ k\ l$  with  $h, k, l$  all even on the other side appeared to vary in the same way with  $l$  (see Table 1), it seemed probable that at least the bismuth atoms are situated on the lines:  $(0\ 0\ 0; \frac{1}{2} \frac{1}{2} 0; 0 \frac{1}{2} \frac{1}{2}; \frac{1}{2} 0 \frac{1}{2}) + 0\ 0\ z$ . The sum of  $\sum_l I_{00l} \cos 2\pi lz$  and  $\sum_l I_{11l} \cos 2\pi lz$  will under such conditions represent the Patterson function along  $0\ 0\ z$ . These two sums are pictured in figure 1. It is seen from the graph that high maxima occur at  $z = 0.144, 0.280$  and  $0.428$ . If  $C_{2h}^{16} c$  is not considered, only the following positions on the lines  $0\ 0\ z$

Table 1  
Weissenberg Photographs of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ . Cu  $K\alpha$  radiation

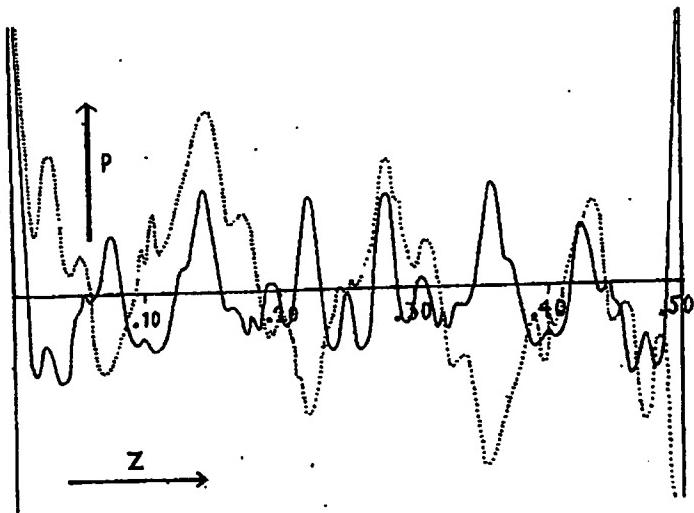
$l$	$I_{\text{calc.}}$	$I_{\text{obs.}}$				$l$	$I_{\text{calc.}}$	$I_{\text{obs.}}$		
		0 0	2 0 or 0 2	2 2	4 2 or 2 4			1 1	3 1 or 1 3	3 3
2	4.4			—	vvv	1	130	vst	m	m
4	20		w	w	—	3	14	w	—	—
6	85	m	m	m	w	5	18	m	vvv	—
8	180	m	m	m	w <sup>+</sup>	7	390	vst	m <sup>+</sup>	m <sup>+</sup>
10	8.4	w	m <sup>-</sup>	vvv	—	9	0.01	—	—	—
12	42	m	m <sup>-</sup>	w	—	11	26	w	vw	vw
14	360	vst	m	m	m	13	42	w	vw	vw
16	3.6	m <sup>+</sup>	—	vvv	—	15	230	w	vw	—
18	32	m <sup>-</sup>	w	vvv	—	17	4.4	—	—	—
20	12	m <sup>-</sup>	w	—	—	19	74	m	vvv	vw
22	260	st	st	m	m	21	300	st	m	w
24	2.0	w	w	vw	—	23	14	m	w	vw
26	110	m	st	st	m <sup>+</sup>	25	37	m	m	w
28	240	m	st	st	st	27	0.09	—	—	—
30	27	w <sup>-</sup>	m	m <sup>-</sup>	m	29	280	st	st	st
32	40	m <sup>-</sup>	st	m	st	31	0.6	w	w	—
34	7.8	vw	w	vw	st	33	150	st	st	st
36	280	m	vst	vst	st	35	170	st	st	st
38	0.1	vw	w	vw	st	37	41	m	m	—
40	190	m	vst	st	st	39	40	st	st	—
42	110	m	st	st	st	41	36	m	—	—

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Figure 1. Patterson function of  $\text{Bi}_4\text{Ti}_3\text{O}_{13}$  along  $00z$ 

$$\text{Full curve: } \sum_l I_{00l} \cos 2\pi lz$$

$$\text{Dotted curve: } \sum_l I_{11l} \cos 2\pi lz \quad (\text{orthorhombic indices})$$

are possible for the Bi atoms: The two 4-fold positions  $000$  and  $00\frac{1}{2}$  and the 8-fold positions  $\pm 00z$ . Assuming that the unit cell contains 16 Bi it was found that the observed maxima in the graph could be explained by assuming that the 16 Bi atoms are situated in two 8-fold positions  $\pm 00z$ . In this way three possibilities arose:

- a.  $z_1 = 0.215 \quad z_2 = 0.356$
- b.  $z_1 = 0.072 \quad z_2 = 0.356$
- c.  $z_1 = 0.072 \quad z_2 = 0.215$ .

If the influence of the Ti and the O atoms is neglected the Patterson maxima will have the following relative weights:

	a	b	c
0.144	2	1	3
0.280	1	3	2
0.428	3	2	1

If the two curves in figure 1 are added and the areas under the peaks calculated, the ratio of  $(0.144):(0.280):(0.428)$  is found to be:  $4.4:2.6:1.0$ . Now, these figures cannot be directly compared with the figures given above, since the zero level in the graph is unknown. It is, however, seen that the observed order of magnitude of the peaks  $(0.144) (0.280)$  and  $(0.428)$  is the same as

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that calculated for c. Case c was therefore assumed, and  $z_1$  and  $z_2$  were varied around 0.072 and 0.215. The observed intensities were found to agree quite well with those calculated for  $z_1 = 0.067 \pm 0.004$  and  $z_2 = 0.211 \pm 0.004$ . In Table I the observed intensities are compared with intensities calculated as follows:  $I = A^2$ ,  $A = 10 (\cos 2\pi l z_1 + \cos 2\pi l z_2) = 10 F/4 f_{\text{Bi}}$ . In Table I the lines of maximum absorption (see (4)) are indicated by dotted lines. If allowance is made for the polarisation factors and the absorption effect (4), it is seen that for  $h, k, l$  all odd the observed and calculated intensities agree quite well. For  $h, k, l$  all even, the calculated ratios of 0016:0018 and 2216:2218 are inverted in comparison with the observed ratios. This might be due to the influence of the Ti and the O atoms.

The calculated intensities may be made to find  $\frac{1}{2}$

Space assumed:

8 F

4 I

## Positions of the Ti atoms

With the formula assumed the unit cell contains 12 Ti atoms. If the space group  $C_{2v}^{16} c$  is not considered, the only 4-fold positions possible are:

- 4 (a)  $x00$  or  $0y0$  ( $C_{2v}^{16} a$  or  $b$ ), 4 (a)  $000$  4 (b)  $00\frac{1}{2}$  ( $D_2^7$ ,  $D_{2h}^{23}$ ),
- 4 (c)  $\frac{1}{2}\frac{1}{2}\frac{1}{2}$  4 (d)  $\frac{1}{2}\frac{1}{2}\frac{1}{2}$  ( $D_2^7$ )

The positions  $000$ ,  $\frac{1}{2}\frac{1}{2}\frac{1}{2}$  and  $\frac{1}{2}\frac{1}{2}\frac{1}{2}$  seemed very improbable since the distance Bi-Ti would then be only 2.2–2.4 Å. For the remaining positions  $00\frac{1}{2}$ ,  $x00$  (or  $0y0$ )  $x$  (or  $y$ ) must lie within the limits 0.38–0.62, if the minimum distance Bi-Ti is assumed to be 3.0 Å. If the distance Ti-Ti is assumed to be  $\geq 3.0$  Å, only 4 Ti can be situated in 4-fold positions and the remaining 8 Ti must occupy one 8-fold position. Of 8-fold positions the following seemed to be possible:

- 8 (d)  $x0z$ ,  $x0\bar{z}$  (or  $0yz$ ,  $0y\bar{z}$ )  $C_{2v}^{16} a$  or  $b$ , 8 (g)  $\pm 00z$  ( $D_2^7$ ,  $D_{2h}^{23}$ ),
- 8 (h)  $\frac{1}{2}\frac{1}{2}z$ ,  $\frac{1}{2}\frac{1}{2}\frac{1}{2}-z$  ( $D_2^7$ )

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Thus there seemed to be two ways of arranging the Ti atoms:

1. 4  $\text{Ti}_1$  in  $00\frac{1}{2}$ , 8  $\text{Ti}_2$  in  $\frac{1}{2}\frac{1}{2}z$ ,  $\frac{1}{2}\frac{1}{2}\frac{1}{2}-z$   $0.133 \leq z \leq 0.147$
2. 4  $\text{Ti}_1$  in  $00\frac{1}{2}$ ,  $x00$  (or  $0y0$ )  $0.38 \leq x \leq 0.62$  (or  $0.32 \leq y \leq 0.68$ )  
8  $\text{Ti}_2$  in  $\pm 00z$   $0.324 \leq z \leq 0.398$ ,  $x0z$ ,  $x0\bar{z}$  (or  $0yz$ ,  $0y\bar{z}$ )  
 $0.38 \leq x \leq 0.62$  (or  $0.38 < y < 0.62$ )  $0.102 \leq z \leq 0.176$

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Both for 1 and 2 the parameters are chosen as to make the distances Bi-Ti  $\geq 3.0$  Å. The region possible for the  $\text{Ti}_2$  atoms — assuming arrangement 2 — is shown by the shaded area in figure 2.

By calculating the intensities of  $00l$  for various  $z_{\text{Ti}}$  values, it was found that the calculated ratio 0016:0018 (see the discussion on the Bi positions) was best for  $z \sim 0.13_0$  or  $0.37_0$ .

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The intensities of the spots in the Weissenberg photographs were then calculated for the arrangements 1 and 2 but no decision between 1 and 2 could be made by comparison with the observed intensities. It was therefore tried to find possible arrangements for the O atoms with both 1 and 2.

## Case 1

Space group  $D_2^T$  and the following positions for the metal atoms were assumed:

8  $\text{Bi}_1$  in 8 (g)  $z_1 = 0.067 \pm 0.004$  8  $\text{Bi}_2$  in 8 (g)  $z_2 = 0.211 \pm 0.004$

4  $\text{Ti}_1$  in 4 (b)  $00\frac{1}{2}$  8  $\text{Ti}_2$  in 8 (h)  $0.133 \leq z \leq 0.147$

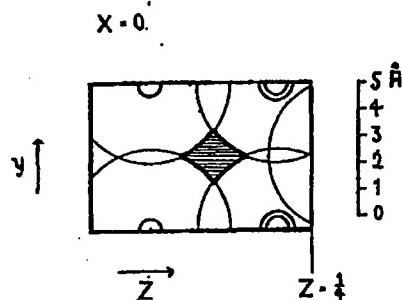


Figure 2.

By assuming that the distances  $\text{Bi}-0 \geq 2.2$ ,  $\text{Ti}-0 \geq 1.8$  and  $0-0 \geq 2.5 \text{ \AA}$ , the following positions were found possible for the O atoms:

$$\begin{array}{lll} 4 \text{ (a)} 000 & 4 \text{ (c)} \frac{1}{2}\frac{1}{2}\frac{1}{2} & 4 \text{ (d)} \frac{1}{2}\frac{1}{2}\frac{1}{2} \\ 8 \text{ (g)} \pm 00z & 8 \text{ (h)} \frac{1}{2}\frac{1}{2}z; \frac{1}{2}\frac{1}{2}\frac{1}{2}-z \\ 0.130 \leq z \leq 0.148 & 0 \leq |z| \leq 0.040 \\ 0.274 \leq z \leq 0.445 & -0.183 \leq z \leq -0.095 \end{array}$$

16 (k)  $xyz; \bar{x}\bar{y}z; \bar{x}y\bar{z}; \bar{x}\bar{y}\bar{z}$

$$\begin{array}{ll} x \approx 0 & y \approx 0 \\ y = 0.27 & x = 0.27 \end{array}$$

Two regions are possible:

$$z = 0.113 \text{ (for } z_{\text{Ti}} = 0.147) \text{ and } z = 0.165 \text{ (for } z_{\text{Ti}} = 0.132)$$

No combinations of these positions could be found giving reasonable distances and octahedra around the Ti atoms, as is the case in previously investigated structures containing  $\text{Ti}^{4+}$  and  $\text{O}^{2-}$ . Arrangement 1 seemed therefore improbable.

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## Case 2

The positions of the metal atoms are assumed to be:

$$8 \text{ Bi}_1 \text{ in } \pm 00z; z_1 = 0.067 \pm 0.004 \quad 8 \text{ Bi}_2 \text{ in } \pm 00z; z_2 = 0.211 \pm 0.004$$

$$4 \text{ Ti}_1 \text{ in } 00\frac{1}{2}, x00 \text{ (or } 0y0) \quad 0.38 \leq x, y \leq 0.62 \quad 8 \text{ Ti}_2 \text{ in } \pm 00z, \\ 0.324 \leq z \leq 0.398$$

$$x0z; x0\bar{z} \text{ (or } 0yz; 0y\bar{z}) \quad 0.38 \leq x, y \leq 0.62 \\ 0.102 \leq z \leq 0.176$$

At first only space group  $D_2^7$  was considered ( $\text{Ti}_1$  in  $00\frac{1}{2}$  and  $\text{Ti}_2$  in  $\pm 00z$ ). The following positions were found possible for the O atoms making the same assumptions as in case 1:

$$4 \text{ (a) } 000$$

$$4 \text{ (c) } \frac{1}{2}\frac{1}{2}\frac{1}{2}$$

$$4 \text{ (d) } \frac{1}{2}\frac{1}{2}\frac{1}{2}$$

$$8 \text{ (g) } \pm 00z$$

$$0.130 \leq z \leq 0.148$$

$$0.379 \leq z \leq 0.445$$

$$0.274 \leq z \leq 0.343$$

$$8 \text{ (h) } \frac{1}{2}\frac{1}{2}z; \frac{1}{2}\frac{1}{2}\frac{1}{2} - z$$

$$0 < |z| < 0.040$$

$$0.095 < |z| < 0.183$$

$$16 \text{ (k) } xyz; x\bar{y}z; x\bar{y}\bar{z}; \bar{x}y\bar{z}$$

$$x = 0.25 \pm 0.02 \quad \text{or} \quad y = 0.25 \pm 0.02$$

$$y \sim 0 \quad x \sim 0$$

$$0.114 < z < 0.163$$

It was tried to find positions for the O atoms so that  $\text{Ti}_1$  and  $\text{Ti}_2$  would be surrounded by regular or almost regular octahedra of O atoms with distances  $1.8 \leq \text{Ti} - \text{O} \leq 2.5 \text{ \AA}$ . For O atoms in contact with  $\text{Ti}_1$ , the following point positions are possible: 8 (h)  $0 < |z| < 0.040$ , 8 (g)  $0.424 \leq z \leq 0.445$ . With 8 O situated at  $\frac{1}{2}\frac{1}{2}0; \frac{1}{2}\frac{1}{2}\frac{1}{2}$  and 8 O at  $\pm 000.442$  regular octahedra of O would surround  $\text{Ti}_1$ . It, therefore, seemed probable that oxygen atoms are situated near these positions.

For oxygen atoms in contact with  $\text{Ti}_2$ , the following positions are possible:

$$8 \text{ (g}_1\text{)} \quad 0.379 \leq z_1 \leq 0.445$$

$$8 \text{ (h) } \quad 0.095 \leq |z| \leq 0.183$$

$$8 \text{ (g}_2\text{)} \quad 0.274 \leq z_2 \leq 0.343$$

$$16 \text{ (k) } \quad 0.114 \leq z \leq 0.163$$

With one set of oxygen atoms situated at 8 (h) or 16 (k), every  $\text{Ti}_2$  atom will be in contact with two oxygen atoms, while if oxygen atoms are situated at 8 (g)<sub>1</sub> or 8 (g)<sub>2</sub>,  $\text{Ti}_2$  will be in contact with only one oxygen atom. It was

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found that only one set of oxygen atoms could occupy the positions 16 (k), 8 (g<sub>1</sub>) and 8 (g<sub>2</sub>), while at most 32 oxygen atoms could be situated in positions 8 (h). The following arrangements allowing Ti<sub>2</sub> to be in contact with 6 O are possible:

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  - a. 16 O (k) + 8 O (h) + 8 O (h)
  - b. 16 O (k) + 8 O (g<sub>1</sub>) + 8 O (g<sub>2</sub>) + 8 (h)
  - c. 8 O (h) + 8 O (h) + 8 O (h)
  - d. 8 O (h) + 8 O (h) + 8 O (g<sub>1</sub>) + 8 O (g<sub>2</sub>)

With a and b no combination of positions could be found, giving octahedra of oxygen atoms around Ti<sub>2</sub>.

c. With 8 O in  $\frac{1}{2}, \frac{1}{2}, 0$ ;  $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ , 8 O in 0 0 0.442 and 24 O in positions 8 (h) ( $z_1 \approx 0.102$   $z_2 \approx -0.139$   $z_3 \approx 0.177$ ) so as to form octahedra of oxygen atoms around Ti<sub>1</sub> and Ti<sub>2</sub>, there was room for the remaining 8 O atoms only in the position  $\pm 0.0z$   $z = 0.274$  or in the positions 4 (c) + 4 (d). With these arrangements, however, the distances O — O would be short ( $\approx 2.4 \text{ \AA}$ ).

With d, positions for the oxygen atoms could be chosen, allowing reasonable distances and giving octahedra of oxygen atoms around Ti<sub>2</sub>. Arrangement d was, therefore, preferred to the arrangements a, b and c.

The following parameters were assumed for oxygen atoms in contact with Ti<sub>1</sub> or Ti<sub>2</sub>:

$$\begin{aligned} & 8 O_1 \text{ in } 8 (h) z = 0 \\ & 8 O_4 \text{ in } 8 (g) z = 0.436 \\ & (z_{Ti_1} = 0.372) \quad 8 O_5 \text{ in } 8 (g) z = 0.308 \\ & \quad 8 O_6 \text{ in } 8 (h) z = 0.128 \\ & \quad 8 O_7 \text{ in } 8 (h) z = -0.128 \end{aligned}$$

Even if these parameters are varied considerably around the values given, room for the remaining 8 O is left only in the positions 4 (c) and 4 (d) (O<sub>2</sub>, O<sub>3</sub>).

The positions arrived at might also be described with space group D<sub>2h</sub><sup>23</sup>—F m m m as follows:

$$\begin{aligned} & 8 O_1 \text{ in } 8 (e) \frac{1}{2}, \frac{1}{2}, 0; \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ & 8 O_8 \text{ in } 8 (f) \frac{1}{2}, \frac{1}{2}, \frac{1}{2}; \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \\ & 8 O_3 \text{ in } 8 (i) \pm 0.0z z = 0.436 \\ & 8 O_4 \text{ in } 8 (i) \pm 0.0z z = 0.308 \\ & 16 O_5 \text{ in } 16 (j) \frac{1}{2}, \frac{1}{2}, z; \frac{1}{2}, \frac{1}{2}, \bar{z}; \\ & \quad \frac{1}{2}, \frac{1}{2}, z; \frac{1}{2}, \frac{1}{2}, \bar{z} \\ & \quad z = 0.128 \end{aligned}$$

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The distances and coordination will be:

$\text{Bi}_1 - 4 \text{ O}_1 = 2.92$	$\text{Ti}_3 - \text{O}_3 = 2.10$	$\text{Ti}_1 - 4 \text{ O}_1 = 1.92$
$\text{Bi}_1 - 4 \text{ O}_3 = 2.72$	$\text{Ti}_2 - \text{O}_4 = 2.10$	$\text{Ti}_1 - 2 \text{ O}_3 = 2.10$
$\text{Bi}_1 - 4 \text{ O}_5 = 2.76$	$\text{Ti}_2 - 4 \text{ O}_5 = 1.92$	
$\text{Bi}_2 - 4 \text{ O}_2 = 2.79$	$\text{O}_1 - 4 \text{ O}_1 = 2.71$	
$\text{Bi}_2 - 4 \text{ O}_4 = 2.79$	$\text{O}_3 - 4 \text{ O}_1 = 2.83$	
$\text{Bi}_2 - 4 \text{ O}_6 = 2.29$	$\text{O}_4 - 4 \text{ O}_2 = 2.70$	
	$\text{O}_4 - 4 \text{ O}_5 = 2.83$	
	$\text{O}_6 - 4 \text{ O}_5 = 2.71$	

No new combinations were found if the space group  $D_{2h}^{22}$  was assumed instead of  $D_2^6$ .

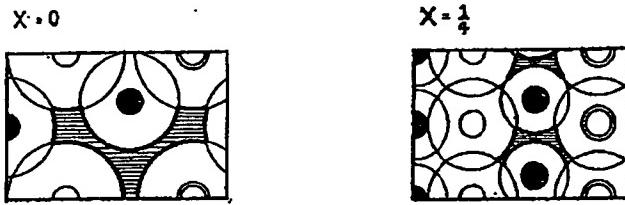


Figure 3 a.

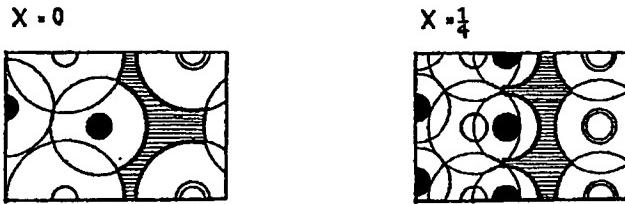


Figure 3 b.

Since  $a \approx b$  and the positions of the O atoms must be chosen from space considerations, it does not matter whether space group  $C_{2h}^{18}$   $a$  or  $b$  is assumed.  $C_{2h}^{18}$   $b$  was assumed arbitrarily. It was found that oxygen atoms could only be situated in the planes  $z=0$ ,  $z=0.25 \pm 0.02$ ,  $z=\frac{1}{3}$  and  $z=0.75 \pm 0.02$ . Thus the following positions are possible:

$$\begin{array}{lll}
 4(a) 0y0 & 8(b) \frac{1}{4}y\frac{1}{4}; \frac{1}{4}y\frac{3}{4} & 8(c) 0yz; 0y\bar{z} \\
 8(d) xy0; \bar{x}y0 & 16(e) xyz; \bar{x}yz; \bar{xy}z; xy\bar{z} & \\
 z = 0.25 \pm 0.02 & & z = 0.25 \pm 0.02
 \end{array}$$

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*Table 2*  
Weissenberg Photographs of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ . Cu  $K\alpha$  radiation

## Zero Layer

$00l$	$I_{\text{calc.}}$	$I_{\text{obs.}}$	$20l$	$I_{\text{calc.}}$	$I_{\text{obs.}}$
6	56	m	2	1.0	vvw
8	61	m	4	12	w
10	12	w	6	59	m
12	58	m	8	81	m
14	450	vst	10	12	vvw
16	88	$m^+$	12	55	w
18	30	m	14	440	m
20	19	m	16	64	vvw
22	200	st	18	31	vvw
24	27	w	20	19	—
26	120	m	22	200	m
28	230	m	24	26	vw
30	62	w	26	120	st
32	140	m	28	230	st
34	4.0	vvw	30	62	m
36	900	m	32	120	vww
38	9.0	vw	34	4.0	vst
40	110	m	36	290	vst
42	93	m	38	8.0	vw
$10l$	$I_{\text{calc.}}$	$I_{\text{obs.}}$	$30l$	$I_{\text{calc.}}$	$I_{\text{obs.}}$
1	52	vst	1	69	m
3	7.0	w	3	8.0	—
5	17	$m^-$	5	18	$m^+$
7	470	vst	7	470	—
9	2.0	—	9	3.0	vw
11	23	w	11	22	vw
13	46	w	13	45	vw
15	120	w	15	130	—
17	23	—	17	21	—
19	98	m	19	93	vw
21	320	st	21	820	w
23	36	m	23	36	vw
25	52	m	25	53	w
27	0.6	—	27	0.8	st
29	270	st	29	270	—
31	19	st	31	19	—
33	110	st			
35	140	st			
37	53	m			
39	75	st			
41	44	m			

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Table 2 (cont.)

First Layer

111	<i>I</i> <sub>calc.</sub>	<i>I</i> <sub>obs.</sub>	311	<i>I</i> <sub>calc.</sub>	<i>I</i> <sub>obs.</sub>
2	1.0	—	2	1.0	—
4	12	w	4	12	—
6	64	m	6	66	w <sup>+</sup>
8	220	m	8	180	w <sup>+</sup>
10	15	m <sup>-</sup>	10	14	—
12	57	m <sup>-</sup>	12	58	—
14	410	m	14	410	m
16	15	—	16	16	—
18	41	w	18	40	—
20	20	w	20	19	—
22	220	st	22	220	m
24	2.0	w	24	3.0	—
26	98	st	26	98	m <sup>+</sup>
28	210	st	28	220	st
30	47	m	30	47	m
32	74	st	32	67	st
34	9.0	w			
36	310	vst			
38	4.0	w			
40	180	vst			
101	<i>I</i> <sub>calc.</sub>	<i>I</i> <sub>obs.</sub>	211	<i>I</i> <sub>calc.</sub>	<i>I</i> <sub>obs.</sub>
5	17	w	1	67	m
7	470	vst	3	8.0	—
9	2.0	vvw	5	18	vvw <sup>+</sup>
11	23	m	7	470	m <sup>+</sup>
13	46	m <sup>+</sup>	9	2.0	—
15	120	m <sup>+</sup>	11	23	vvw
17	23	w <sup>+</sup>	13	46	vvw
19	98	m <sup>+</sup>	15	130	vvw
21	320	st	17	22	—
23	36	m	19	96	vvw
25	52	m	21	320	m
27	0.6	—	23	36	w
29	270	st	25	50	m
31	19	w	27	0.8	—
33	110	st	29	270	st
35	140	st	31	19	w
37	53	m	33	110	st
39	75	st	35	140	st
41	44	st	37	53	m

POW<sub>C</sub>

0	1	1	—
1	1	—	1
2	0	0	0
3	0	0	0
4	0	0	0
5	0	0	0
6	0	0	0
7	0	0	0
8	0	0	0
9	0	0	0
10	0	0	0
11	0	0	0
12	0	0	0
13	0	0	0
14	0	0	0
15	0	0	0
16	0	0	0
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25	0	0	0
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28	0	0	0
29	0	0	0
30	0	0	0
31	0	0	0
32	0	0	0
33	0	0	0
34	0	0	0
35	0	0	0
36	0	0	0
37	0	0	0
38	0	0	0
39	0	0	0
40	0	0	0
41	0	0	0

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Table 3

Powder Photographs of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ . Cr  $K$  radiation, orthorhombic description

$hkl$	$10^4 \sin^2 \theta_{\text{calc.}}$	$10^4 \sin^2 \theta_{\text{obs.}}$	$I_{\text{obs.}}$	$hkl$	$10^4 \sin^2 \theta_{\text{calc.}}$	$10^4 \sin^2 \theta_{\text{obs.}}$	$I_{\text{obs.}}$
0 0 8	0779	0771	st	1 1 19	5282	5292	m
1 1 1	0903	0895	m	2 2 12	5314		
1 1 5	1195	1188	vvw	0 2 18	5710	5734	vww
—	—	1288	m-	2 0 18	5735		
—	—	1396	w	0 0 22	5887	5892	m
1 1 7	1487	1480	vst	1 3 11	5900	5949	m
—	—	1614	vw	2 2 14	5946		
0 0 12	1752	1762	m	3 1 11	5950		
0 2 0	1769			1 1 21	6255	6267	st
2 0 0	1794	1790	w	0 2 20	6635	6664	vw
0 2 4	1964	1952	vw	2 0 20	6660		
$\beta$ 0 0 14	1974	1974	m-	2 2 16	6676		
2 0 4	1989			0 4 0	7074	7070	vw
0 0 14	2384	2384	vst	1 3 15	7165	7172	m
0 2 8	2548	2585	st	4 0 0	7174		
2 0 8	2573			3 1 15	7215	7221	m-
1 1 13	2947	2947	m	4 0 2	7223		
$\beta$ 2 2 0	2953			1 1 23	7326	7335	w
0 2 10	2985			2 2 18	7503	7511	w
$\beta$ 1 1 15	3003	3005	w	0 4 6	7512		
2 0 10	3010			0 2 22	7656	7674	m
0 0 16	3114	3115	m-	2 0 22	7681		
0 2 12	3521	3538	vww	1 1 25	8494	8495	w w
2 0 12	3546			3 3 7	8611	8611	m
2 2 0	3562	3567	m	2 0 24	8801		
1 1 15	3628	3638	m	1 3 19	8819	8806	vw
0 0 18	3941	3942	w	0 4 12	8826		
2 2 6	4000	4006	w	2 4 0	8868		
0 2 14	4153			3 1 19	8869	8859	w
$\beta$ 1 3 7	4159	4171	st	2 4 2	8917		
2 0 14	4178			4 0 12	8926	8934	vw
$\beta$ 3 1 7	4200			4 2 0	8943		
2 2 8	4341	4333	w	2 2 22	9449	9458	st
1 1 17	4406	4418	vww	0 4 14	9458		
1 3 1	4440	4428	vww	0 0 28	9537	9551	m
3 1 1	4482	4490	vww	4 0 14	9558		
0 0 20	4866	4880	w	2 4 8	9647	9652	vw
0 2 16	4883			4 2 8	9722	9714	vw
2 0 16	4908	4923	w	1 3 21	9792	9785	w
$\beta$ 2 2 14	4922						
1 3 7	5024	5029	m				
3 1 7	5074	5078	m				

The positions of the Ti atoms are assumed to be:

$$4 \text{ Ti}_1 \text{ in } 4 \text{ (a)} \quad 0.38 \leq y_1 \leq 0.62$$

$$8 \text{ Ti}_2 \text{ in } 8 \text{ (c)} \quad 0.38 \leq y_2 \leq 0.62 \quad 0.102 \leq z_2 \leq 0.176$$

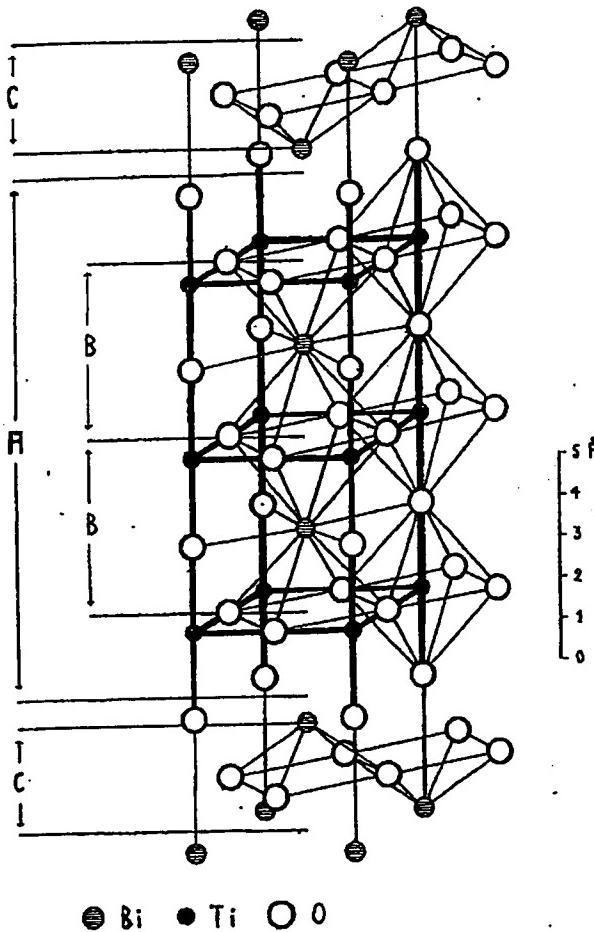
B. AURIVILLIUS, *Mixed bismuth oxides with layer lattices. II*

Figure 4.

One half of the pseudo-tetragonal unit cell of  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  (from  $z \approx 0.25$  to  $z \approx 0.75$ ). A denotes the perovskitic layer  $\text{Bi}_3\text{Ti}_3\text{O}_{12}^+$ , C  $\text{Bi}_3\text{O}_3^{3+}$  layers and B unit cells of the hypothetical perovskite structure  $\text{BiTiO}_3$ .

In figures 3 a and 3 b sections of one fourth of the unit cell are made for  $z = 0$  and  $z = 0.25$ . (The projections of the positions of the  $\text{Bi}_1$ ,  $\text{Bi}_2$  and  $\text{Ti}$  atoms are denoted by: white circles, double circles and black circles respectively. The same scale is used as for figure 2). Regions where oxygen atoms might be situated are shown by shaded areas. In figure 3 a the positions of the  $\text{Ti}$  atoms are assumed to be:  $0 0 \frac{1}{2}$  and  $0 y z$ ;  $0 y \bar{z}$   $y = 0.62$   $z = 0.139$  and in figure 3 b,  $0 y 0 y = 0.62$  and  $\pm 0 z z = 0.324$ .

As in the discussion above it was tried to find positions for the  $\text{O}$  atoms giving an octahedral arrangement around  $\text{Ti}_1$  and  $\text{Ti}_2$ . Only with  $\text{O}$  atoms situated in the positions 8 (d)  $x \approx \frac{1}{4}$   $y \approx y_1 + \frac{1}{4}$  and 8 (c)  $y \approx y_1$   $z \approx 0.058$  would  $\text{Ti}_1$  be surrounded by regular octahedra (see figure 3). It was therefore assumed that these positions are occupied by oxygen atoms. For oxygen atoms in contact with  $\text{Ti}_2$ , the point positions 8 (c) and 16 (e) are possible. With 8  $\text{O}$  situated at 8 (c), every  $\text{Ti}$  atom is in contact with one oxygen atom; with 16  $\text{O}$  in 16 (e),  $\text{Ti}_2$  may be in contact with 2  $\text{O}$  (e<sub>2</sub>) or 4  $\text{O}$  ( $y \approx y_2 + \frac{1}{4}$   $z \approx z_2$ ) (e<sub>4</sub>). Bear-

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ing in mind that the unit cell contains 48 O and assuming 16 O to be situated at 8 (c) + 8 (d) (so as to form an octahedron around  $Ti_1$ ), the following arrangements giving 6 O around  $Ti_2$  seemed possible:

- a. 8 O (c) + 8 O (c) + 16 O (e<sub>4</sub>)
- b. 16 O (e<sub>2</sub>) + 16 O (e<sub>4</sub>).

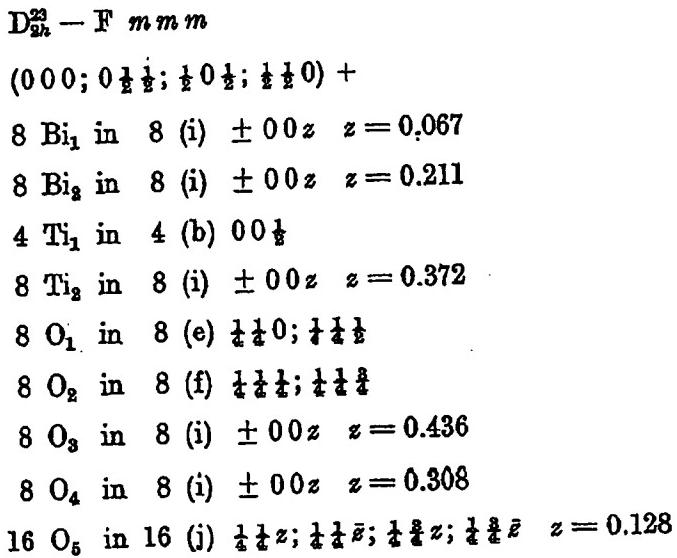
With b. no combination giving octahedra of O around  $Ti_2$  could be found. With a., however, arrangements could be found allowing  $Ti_2$  to be surrounded by an almost regular octahedron. The following parameters for oxygen atoms in contact with  $Ti_1$  or  $Ti_2$  were assumed:

$$\begin{aligned} 8 O_1 \text{ in } 8 (d) \quad & x = \frac{1}{4} \quad y \approx y_1 + \frac{1}{4} \\ 8 O_2 \text{ in } 8 (c) \quad & y \approx (y_1 + y_2)/2 \quad z \approx z_2/2 \\ 8 O_3 \text{ in } 8 (c) \quad & y \approx y_2 \quad z \approx 3z_2/2 \\ 16 O_4 \text{ in } 16 (e) \quad & x = \frac{1}{4} \quad y \approx x_2 + \frac{1}{4} \quad z \approx z_2 \end{aligned}$$

For the remaining 8 O there seemed to be room only in the position 8 (b)  $y \approx \frac{1}{4}$ . It is seen that these positions are basically the same as were arrived at when space group  $D_{2h}^T$  was assumed, except for possible small shifts in the  $y$  direction.

Thus no new arrangement was found by assuming  $C_{2h}^{16}$  a or b. In Table 2 (pseudo-tetragonal indices) the intensities, calculated by means of the formula  $I = (10 F/4 f_B)^2$ , are compared with the observed ones. Since the ratios  $f_{Ti}/f_B$  and  $f_O/f_B$  vary with  $\sin \theta/\lambda$  they were interpolated for every reflection from values taken from the International Tables (3). Table 2 shows good agreement between the calculated and observed intensities.

The following structure is thus proposed:



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For the pseudo-tetragonal cell the positions will be:

$D_{\text{th}}^{17} - I \ 4/m \ m \ m$   
 $(000; \frac{1}{2} \frac{1}{2} \frac{1}{2}) +$   
 4  $\text{Bi}_1$  in 4 (e)  $\pm 00z$   $z = 0.067$   
 4  $\text{Bi}_2$  in 4 (e)  $\pm 00z$   $z = 0.211$   
 2  $\text{Ti}_1$  in 2 (b)  $00\frac{1}{2}$   
 4  $\text{Ti}_2$  in 4 (e)  $\pm 00z$   $z = 0.372$   
 4  $\text{O}_1$  in 4 (c)  $0\frac{1}{2}0; \frac{1}{2}00$   
 4  $\text{O}_2$  in 4 (d)  $0\frac{1}{2}\frac{1}{2}; \frac{1}{2}0\frac{1}{2}$   
 4  $\text{O}_3$  in 4 (e)  $\pm 00z$   $z = 0.436$   
 4  $\text{O}_4$  in 4 (e)  $\pm 00z$   $z = 0.308$   
 8  $\text{O}_5$  in 8 (g)  $\pm (0\frac{1}{2}z; \frac{1}{2}0\bar{z})$   $z = 0.128$

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In figure 4 one half of the pseudo-tetragonal unit cell is pictured. The structure consists of  $\text{Bi}_2\text{O}_3^{2+}$  layers alternating with  $\text{Bi}_2\text{Ti}_3\text{O}_{10}^{2-}$  layers. The arrangements of the atoms within the  $\text{Bi}_2\text{Ti}_3\text{O}_{10}^{2-}$  layers seems to be the same as that found for perovskite structures, and it is easily found by calculation that the geometrical properties of the  $\text{Bi}^{3+}$ ,  $\text{Ti}^{4+}$  and  $\text{O}^{2-}$  ions make a perovskite structure possible. Thus the structure might be looked upon as a layer structure where perovskitic layers  $\text{Bi}_2\text{Ti}_3\text{O}_{10}^{2-}$  — corresponding to a hypothetical perovskite structure  $\text{BiTiO}_3$  — alternate with  $\text{Bi}_2\text{O}_3^{2+}$  layers. With the notations given by LAGERCRANTZ and SILLÉN (5), the above structure might be denoted by XIII.

I wish to thank Professor L. G. SILLÉN for valuable discussions concerning this work.

Stockholms Högakola, Institute of Inorganic and Physical Chemistry, 1949.

REFERENCES. 1. Bannister, F. A. and Hey, M. H., Miner. Mag. 24 (1935), 49. —  
 2. Sillén, L. G., Dissert. Stockholm 1940. — 3. Internationale Tabellen zur Bestimmung von Kristallstrukturen, Berlin 1935. — 4. Wells, A. F., Z. Krist. 96 (1937), 451. —  
 5. Lagercrantz, Å. and Sillén, L. G., Arkiv f. Kemi etc. 25 (1947), 49.

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Tryckt den 10 januari 1950

Uppsala 1950. Almqvist & Wiksell's Boktryckeri AB

**BRIEF ATTACHMENT X**

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of

Applicants: Bednorz et al.

Serial No.: 08/479,810

Filed: June 7, 1995

For: **NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION**

Date: March 1, 2005

Docket: YO987-074BZ

Group Art Unit: 1751

Examiner: M. Kopeć

Commissioner for Patents  
P.O. Box 1450  
Alexandria, VA 22313-1450

**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the following:

**ATTACHMENT X**

## ARKIV FÖR KEMI Band 2 nr 37

Communicated 24 May 1950 by ARNE WESTGREN and PERCY QUENSEL

## Mixed oxides with layer lattices

III. Structure of  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ 

By BENGT AURIVILLIUS

With 4 figures in the text

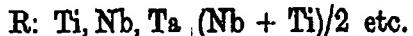
X ray studies on the compounds  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  (1) and  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  (2) have shown that the comparatively complicated chemical formulae of these compounds can be explained by simple layer structures being built up from  $\text{Bi}_2\text{O}_3^{2+}$  layers and perowskite layers. The unit cells are pictured schematically in Figs. 1 a and 1 c. It was found both for  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  and  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  that the symmetry was body-centered pseudo-tetragonal and that the length of the  $a$  axes had the same value ( $3.8 \text{ \AA}$ ) while the length of the  $c$ -axis was  $25 \text{ \AA}$  for  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  and  $33 \text{ \AA}$  for  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ . In both structures the heavy atoms form approximately a "substructure" with a smaller body-centered tetragonal cell with  $a = 3.8 \text{ \AA}$  and  $c = 25/5 \text{ \AA}$  for  $\text{CaBi}_2\text{Nb}_2\text{O}_9$ , or  $c = 33/7 \text{ \AA}$  for  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ .

The  $\text{Bi}_2\text{O}_3$  layers and perowskite layers lie perpendicular to the  $c$ -axis. Similar layer structures have been found for a number of bismuth oxides (3,4,5). The common structural element in all these compounds is quadratic  $\text{Bi}_2\text{O}_3$  layers between which halides or certain radicals are inserted. This explains the fact that the  $a$  axes of all these compounds are of about the same length. For a survey see (5).

For the  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  type each perowskite layer has the composition  $(\text{CaNb}_2\text{O}_7)_n$  and the height of the layer is equal to four distances  $\text{Nb}-\text{O}$  or approximately to the height of two  $\text{E}2_1$  (perowskite) unit cells (see Fig. 1 a). A compound with a somewhat similar structure has previously been investigated by LAGERCRANTZ and SILLÉN (5). In this structure (see Fig. 1 b), beyerite  $\text{CaBi}_2\text{O}_2(\text{CO}_3)_2$ , the point positions corresponding to the positions of the  $\text{Nb}$  atoms in  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  are occupied by "rotating"  $\text{CO}_3^{2-}$  groups.

For the  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  type the perowskite layers have the composition  $(\text{Bi}_2\text{Ti}_3\text{O}_{10})_n$  and the height of the layer is equal to six distances  $\text{Ti}-\text{O}$  or approximately to the height of three  $\text{E}2_1$  unit cells.

The general formula for a compound built up in a way similar to  $\text{CaBi}_2\text{Nb}_2\text{O}_9$  but where the height of the perowskite layer enclosed between a pair of  $\text{Me}_2\text{O}_3$  layers is equal to the height of  $m$   $\text{E}2_1$  cells, will be:



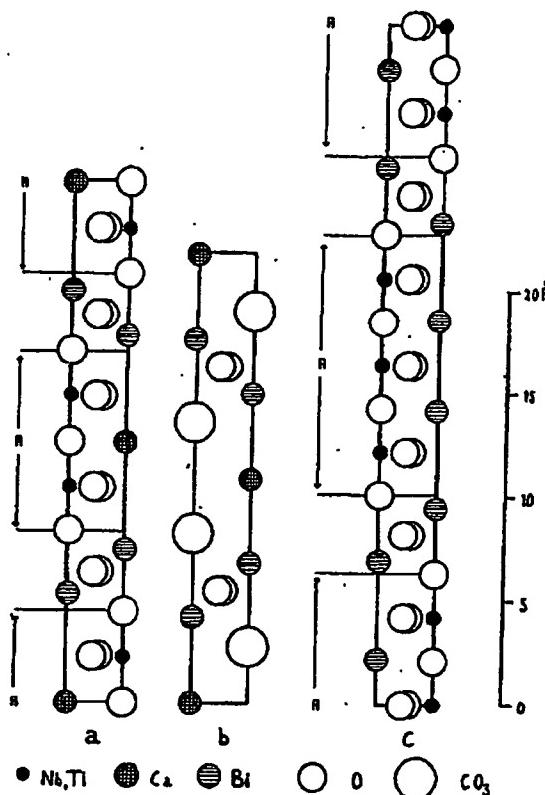
B. AURIVILLIUS, *Mixed oxides with layer lattices. III.*

Fig. 1. Schematic pictures of the structures of a.  $\text{CaBi}_2\text{Nb}_2\text{O}_9$ , b.  $\text{CaBi}_2\text{O}_8(\text{CO}_3)_2$ , and c.  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ . The vertical lines indicate the lines  $00z$  and  $\frac{1}{2}\frac{1}{2}z$  in the unit cells. A denotes perovskitic ( $\text{E}_{21}$ ) regions in the structures.

It seemed of interest to investigate whether compounds could be synthesized with  $m = 4$ . The present investigation shows that structures of the above type with  $m = 4$  exist.

Mixtures of  $\text{Bi}_2\text{O}_3$ ,  $\text{BaCO}_3$  and  $\text{TiO}_2$ , corresponding to the composition  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ , were prepared and heated to  $1100^\circ\text{C}$ . Single crystals, thin plates, were picked out and Weissenberg photographs were taken. These could be interpreted by means of a body-centered tetragonal cell with  $a = 3.86 \text{ \AA}$  and  $c = 41.7 \text{ \AA}$ . The strong lines of the powder photographs (taken from preparations heated to  $900^\circ\text{C}$  (Au crucible) or  $1100^\circ\text{C}$  (Pt crucible)) were easily identified since they could all be described with the aid of the "sub-lattice" ( $a = 3.86 \text{ \AA}, c = 41.7/9$ ). If the  $c$  axis were 9 fold even the weak lines could be explained (Table 3). In this way the cell edges were found to be  $a = 3.864 \text{ \AA}$  and  $c = 41.76 \text{ \AA}$ . The observed density was 7.2, which agrees fairly well with the assumption of 2 formula units/unit cell (calculated density 7.49).

The Weissenberg photographs registered  $0kl$ ,  $1kl$ ,  $hhl$  and  $h, h+1, l$ . In the Weissenberg and powder photographs there was nothing to indicate a lower Laue symmetry than  $D_{4h} - 4/mmm$ . Except for the extinctions due to the body-centering,  $hkl$  occurring only for  $h+k+l=2n$ , no systematic extinctions were found, which is characteristic of the space groups  $C_{4v}^0$ ,  $D_{2h}^{11}$  and  $D_{4h}^{17}$ . Fig. 2

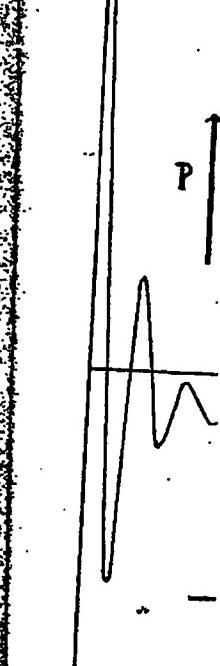


Fig. 2. Patterson

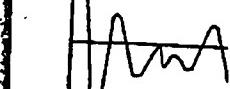


Fig. 3. Three dim. material was used  
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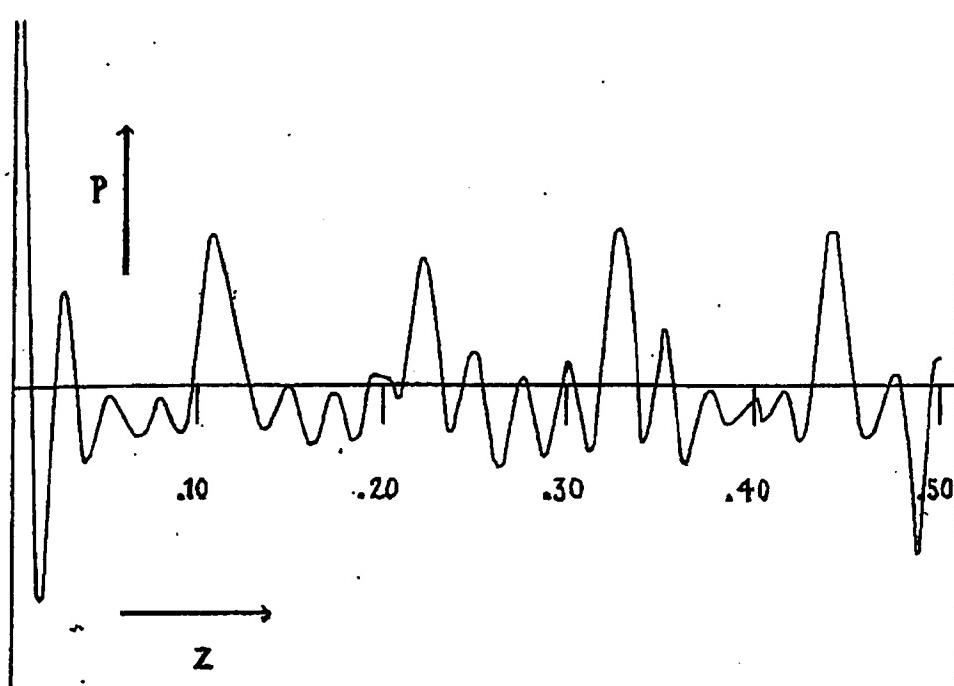


Fig. 2. Patterson Harker function of  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$  along  $00z$ . All observed reflexions were used for this calculation.

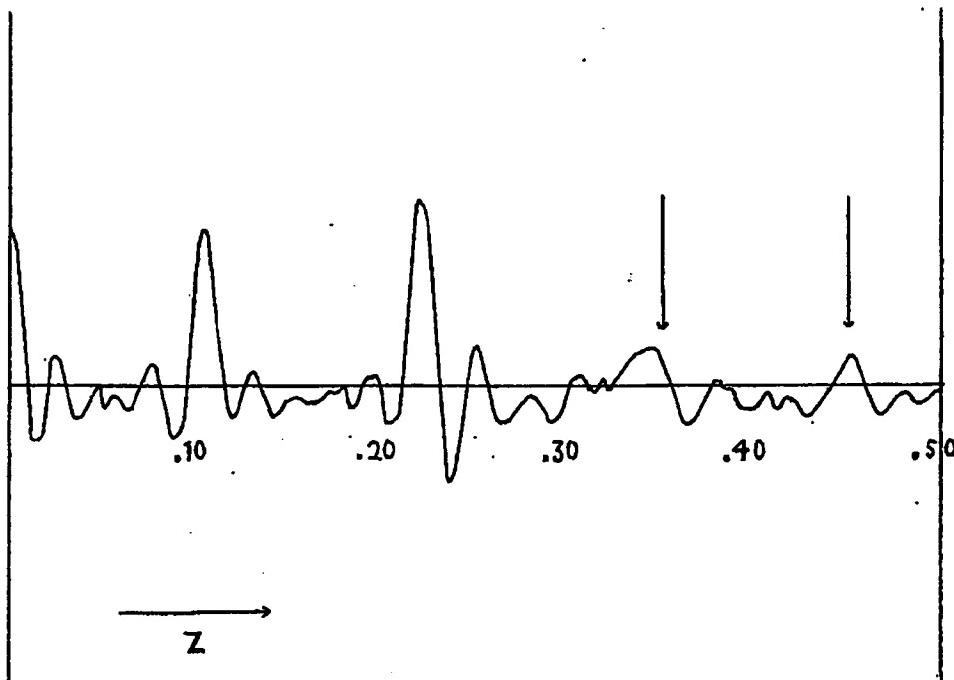


Fig. 3. Three dimensional Fourier cut along  $00z$  for  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ . The same intensity material was used as for the Patterson Harker analysis pictured in Fig. 2. The signs of the amplitudes are the same as those obtained in the structure factor calculation for Table 2.

The vertical arrows correspond to the  $z_{\text{Ti}}$  values actually assumed.

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shows the Patterson Harker function along  $00z$ . For all observed reflexions the  $F^2$  values were estimated from:  $F^2 \approx I_{\text{obs}} \frac{\sin 2\theta}{1 + \cos^2 2\theta}$ . As expected large peaks appear at  $z \approx 1/9, 2/9, 3/9$  and  $4/9$ .

It is interesting to compare the cell dimensions found above with the ones which might be expected if the compound  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$  is assumed to have a structure similar to that of  $\text{CaBi}_2\text{Nb}_2\text{O}_9$ , but with  $m = 4$ . In this case the  $a$  axis would have about the same value as found. The length of the  $c$  axis might be estimated in the following way: The  $c$  axis of  $\text{Bi}_3\text{NbTiO}_9$  ( $m = 2$  see (1)) is  $25.11 \text{ \AA}$ ; the value for  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  ( $m = 3$  see (2)) is  $32.83$ , the difference is  $7.72$ . If twice this value is added to the  $c$  axis of  $\text{BaBi}_2\text{Nb}_2\text{O}_9$  ( $m = 2$ ) the value  $41.0 \text{ \AA}$  is obtained. The value actually found was, as mentioned above,  $41.76 \text{ \AA}$ .

From the composition, cell dimensions, and crystal symmetry it seemed *a priori* probable that the structure of  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$  was the one we anticipated. Therefore, the parameters were worked out with the aid of the parameters found for

Table 1

Weissenberg photographs of  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ . Cu  $K\alpha$  radiation. For zero order photographs the regions of maximum absorption (see Wells (6)) are indicated by dotted lines. The intensities of 101, 103 and 105 have been taken from a zero order photograph, those of 1027–1049 from a first order photograph rotated around (100).

$l$	0 0 1	2 0 1	2 2 1	4 0 1	1 1 1	3 1 1	3 3 1
2		—	vw	—	—	—	vw
4		—	—	—	vw	—	vww
6	vw	vww	vw	—	w	—	vww
8	m	m	w	—	m	vww	vww
10	m	m	w	—	st	vw	w
12	w	vww	vw	—	vww	—	w
14	w	—	vww	—	w	—	—
16	st	w	m <sup>+</sup>	vww	m	vww	m
18	vst	m	st	w	vst	w	st
20	st	w	w	vww	w	—	—
22	m <sup>+</sup>	vww	vww	vww	vw	—	vw
24	w	vww	vww	vww	vw	—	w
26	w	vww	—	—	w	vww	w
28	st	m <sup>+</sup>	w <sup>+</sup>	m	m	vw	—
30	w	w	w	m <sup>+</sup>	—	vw	—
32	w	w <sup>+</sup>	w <sup>+</sup>	—	m	w	—
34	m	m	m <sup>+</sup>	—	m	m	—
36	st	st	st	—	m <sup>+</sup>	m	—
38	vww	—	—	—	w	—	—
40	st	st	st	—	st	st	—
42	vww	—	—	—	vw	—	—
44	—	—	—	—	—	—	—
46	m	m	m	—	st	st	—
48	w	w <sup>+</sup>	w <sup>+</sup>	—	st	st	—
50	w <sup>+</sup>	w <sup>+</sup>	w <sup>+</sup>	—	m	—	—
52	w	w <sup>+</sup>	w <sup>+</sup>	—	—	—	—

$\text{Bi}_3\text{NbTiC}$   
to be: 2  
The pc

4 Ti in :  
 $\frac{1}{2} 0 (\frac{1}{2} - z_3)$   
4 O in  $\pm$   
 $z_1 \approx 1/9$

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Table I (cont.)

Weissenberg photographs of  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ . Cu  $K_{\alpha}$  radiation.

$l$	101	211	301	321	411
1	m	w	vw	vw	—
3	vvv	vvv	—	vvv	—
5	vvv	—	—	—	—
7	w	vw	vvv	w	—
9	st	st	m	m	w
11	—	—	—	—	—
13	w	—	—	—	—
15	w <sup>+</sup>	—	vvv	—	—
17	m	vvv	vvv	—	—
19	st	vw	vvv	vvv	vvv
21	w	—	vvv	vvv	vvv
23	w <sup>+</sup>	—	vvv	vvv	m
25	m <sup>+</sup>	vw	vw	vw	m <sup>+</sup>
27	st	m	w	m	—
29	m	vw	vvv	vvv	—
31	m	w	vw	vw	—
33	vw	vvv	vvv	vw	—
35	—	—	—	—	—
37	m <sup>+</sup>	m	m	—	—
39	vw	w	m	—	—
41	w	w	w <sup>+</sup>	—	—
43	w <sup>+</sup>	m	—	—	—
45	m	m <sup>+</sup>	—	—	—
47	—	—	—	—	—
49	st	—	—	—	—
51	—	—	—	—	—

$\text{Bi}_3\text{NbTiO}_9$  and  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ . The positions of the heavy atoms might be expected to be: 2 Ba in 000, 4 Bi in  $\pm 00z_1$ , 4 Bi in  $\pm 00z_2$ .

The positions of the Ti and O atoms might be expected to be:

4 Ti in  $\pm 00z_3$ , 4 Ti in  $\pm 00z_4$ , 2 O in  $00\frac{1}{2}$ , 8 O in  $\pm (0\frac{1}{2}(\frac{1}{2}-z_3))$ ,  $\pm 0(\frac{1}{2}-z_3)$ , 8 O in  $\pm (0\frac{1}{2}(\frac{1}{2}-z_4))$ ,  $\pm 0(\frac{1}{2}-z_4)$ , 4 O in  $\pm 00(z_3+z_4)/2$ , 4 O in  $\pm 00(z_3-(z_4-z_3)/2)$ , 4 O in  $0\frac{1}{2}\frac{1}{2}, \pm 0\frac{1}{2}$

$$z_1 \approx 1/9 \quad z_2 \approx 2/9 \quad z_3 \approx 0.350 \quad z_4 \approx 0.450$$

These atomic positions would give rise to high peaks in the Patterson-Harker plot at the same values as actually found. The calculated area ratios agree, however, with the observed ones only in as much as the biggest area is found for the peak at 1/9. The reasons might be an incorrect choice of the zero level and errors in the estimation of the intensities.

The parameters were varied around the above values for different positions of the Ba atoms: 2 Ba in 000,  $00z_1$  or  $00z_2$ , 2 Ba equally distributed over  $(000+00z_1)$ ,  $(000+00z_2)$ ,  $(00z_1+00z_2)$  or  $(000+00z_1+00z_2)$ . The best agreement seemed to be for  $z_1 = 0.106 \pm 0.001$ ,  $z_2 = 0.221 \pm 0.001$ ,  $z_3 = 0.352 \pm 0.004$ ,  $z_4 = 0.452 \pm 0.004$  with 2 Ba equally distributed over  $(000+00z_1+00z_2)$ .

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Table 2

Weissenberg photographs of  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ . Cu  $K\alpha$  radiation  
 $I_{\text{calc.}} = (2.5 F/f_{\text{Bi}})^2$

$l$	$I_{\text{obs.}}$ 1 0 1	$I_{\text{calc.}}$ 1 0 1	$I_{\text{obs.}}$ 2 1 1	$I_{\text{calc.}}$ 2 1 1	$I_{\text{obs.}}$ 3 0 1	$I_{\text{calc.}}$ 3 0 1	$h \ k \ l$
1	m	73	w	90	vw	94	0 0 10
3	vvv	5.8	vvv	7.3	—	8.4	1 0 1
5	vvv	4.8	—	5.8	—	5.8	1 0 5
7	w	30	vw	31	vvv	32	1 0 9
9	vst	620	st	610	m	630	1 1 0
11	—	13	—	12	—	14	0 0 16
13	w <sup>+</sup>	25	—	24	—	24	1 1 6
15	w <sup>+</sup>	62	—	60	vvv	60	1 1 8
17	m	94	vvv	92	vvv	90	0 0 18
19	st	160	vw	170	vvv	170	1 1 10
21	w	15	—	12	vvv	12	1 0 15
23	w <sup>+</sup>	19	—	18	vvv	18	0 0 20
25	m <sup>+</sup>	120	vw	120	vw	120	1 0 17
27	st	820	m	320	w	320	2 0 0
29	m	45	vw	45	vvv	44	1 0 19
31	m	160	w	160	vw	160	1 1 16
33	vw	56	vvv	56	vvv	56	2 0 8
35	—	13	—	12	—	12	{ 1 1 18
37	m <sup>+</sup>	300	m	300	m	300	{ 1 0 21
39	vw	12	w	13	m <sup>+</sup>	13	{ 2 0 10
41	w	15	w	14	w <sup>+</sup>	15	{ 2 1 1
43	w <sup>+</sup>	200	m <sup>+</sup>	200	—	—	{ 2 1 3
45	m	180	m <sup>+</sup>	180	—	—	{ 2 1 7
47	—	18	—	—	—	—	{ 1 1 20
49	st	250	—	—	—	—	{ 2 0 14
51	—	3.6	—	—	—	—	{ 2 1 9
$l$	$I_{\text{obs.}}$ 0 0 1	$I_{\text{calc.}}$ 0 0 1	$I_{\text{obs.}}$ 1 1 1	$I_{\text{calc.}}$ 1 1 1	$I_{\text{obs.}}$ 2 2 1	$I_{\text{calc.}}$ 2 2 1	
2	—	—	—	0.5	vw	0.6	00z <sub>2</sub> ). Oth
4	vw	21	vw	4.8	—	5.8	seen the thi
6	m	110	w	23	vw	24	following M
8	m	62	st	100	w	110	over the po
10	w	12	vvv	280	w	98	From Tal
12	w	14	w	6.3	vw	9.6	= I <sub>221</sub> ≈ I <sub>4</sub>
14	st	83	m	16	vvv	14	be expected
16	vst	440	vst	79	m <sup>+</sup>	81	00z, $\frac{1}{2}\frac{1}{2}z$ ,
18	st	170	w	480	st	450	for the rows
20	st	100	vw	36	w	120	senberg pho
22	m <sup>+</sup>	81	vw	79	vvv	92	the observed
24	w	39	w	86	vvv	78	more clearly
26	st	280	m	36	—	39	≥ 3039. Th
28	w	2.6	—	240	w	280	the z param
30	w	11	—	11	w	1.4	structure fac
32	m	140	m	20	w	12	are 222:22.
34	st	240	m <sup>+</sup>	110	m <sup>+</sup>	140	reflexions the
36	vvv	19	w	240	st	240	be introduced
38	st	380	st	35	—	21	the agreemen
40	vww	11	vw	280	st	340	
42	—	3.2	—	22	—		
44	m	240	st	4.8	—		
46	w	69	st	230	—		
48	w <sup>+</sup>	53	m	46	—		
50	w <sup>+</sup>	280	—	110	—		
52	w <sup>+</sup>	—	—	—	—		

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Table 3

Powder photographs of BaBi<sub>4</sub>Ti<sub>4</sub>O<sub>15</sub> Cr K<sub>α</sub> radiation.

alc. 0 1	$h k l$	$10^4 \sin^2 \theta_{\text{calc.}}$	$10^4 \sin^2 \theta_{\text{obs.}}$	$I_{\text{obs.}}$	$h k l$	$10^4 \sin^2 \theta_{\text{calc.}}$	$10^4 \sin^2 \theta_{\text{obs.}}$	$I_{\text{obs.}}$
34	0 0 10	753	745	w	2 0 16	5443	5440	vw
8.4	1 0 1	887	878	m	1 0 25	5582	5581	w
5.8	1 0 5	1067	1058	vw	2 1 13	5667	5669	vvw
32	1 0 9	1489	1481	st	0 0 28	5900	5892	vw
30	1 1 0	1758	1751	m	2 0 18	5954	5960	m
14	0 0 16	1927	1915	vvw	{ 2 1 15	6088	6089	vw
24	1 1 6	2031	2018	vw	{ 1 1 24	6093	6089	vw
80	1 1 8	2240	2236	vw	1 0 27	6365	6364	m
90	0 0 18	2438	2423	m	2 0 20	6526	6529	vw broad
70	1 1 10	2611	2504	m <sup>+</sup>	{ 2 2 0	7032		
12	1 0 15	2572	2567	vvw	{ 2 2 2	7064	7070	w broad
18	0 0 20	3010	2992	w	{ 2 1 19	7112		
20	1 0 17	3054	3051	w	{ 3 0 5	8099		
20	2 0 0	3518	3514	m	{ 1 0 31	8111	8104	vvw
44	1 0 19	3696	3600	w <sup>+</sup>	{ 2 2 14	8114		
60	1 1 16	3685	3681	w	{ 2 1 23	8376	8365	vw
58	2 0 8	3998	3996	vw	{ 2 2 14	8507		
12	{ 1 1 18	4196	4186	m	{ 3 0 9	8521	8520	m
00	{ 1 0 21	4198	4186	m	{ 1 1 30	8531		
13	2 0 10	4269	4265	w	{ 3 1 0	8802		
15	{ 2 1 1	4403	4402	vw	{ 3 0 11	8812	8802	m
	{ 2 1 3	4418			{ 3 1 2	8820		
	{ 2 1 7	4764	4774	vw	{ 1 0 33	9074		
	{ 1 1 20	4768	4774	vw	{ 2 1 25	9098	9092	w broad
	{ 2 0 14	4991			{ 1 1 32	9464	9484	w broad
	{ 2 1 9	5005	5009	m <sup>+</sup>	{ 2 2 18	9470		

00z<sub>2</sub>). Other distributions of Ba should, however, not be excluded; as will be seen the three dimensional Fourier cut along 00z (see Fig. 3) seems to favour the following Me arrangement: 4 Bi  $\pm$  00z<sub>2</sub> and (2 Ba + 4 Bi) equally distributed over the positions 000 and  $\pm$  00z<sub>1</sub>.

From Table 1 it is seen that roughly for the same value of  $l$ :  $I_{00l} \approx I_{20l}$   
 $\approx I_{22l} \approx I_{40l}$ ,  $I_{11l} \approx I_{31l} \approx I_{33l}$ ,  $I_{10l} \approx I_{21l} \approx I_{30l} \approx I_{32l} \approx I_{41l}$  as might be expected from the above atomic positions with atoms only on the lines 00z,  $\frac{1}{2}\frac{1}{2}z$ ,  $0\frac{1}{2}z$  and  $\frac{1}{2}0z$ . Table 2 gives calculated and observed intensities for the rows 00l, 10l, 11l, 21l, 22l and 30l. It was found from the Weissenberg photographs that  $0028 \gg 0030$  and  $1037 > 1039$  (see Table 2) but the observed ratios do not seem to be as large as those calculated. This is more clearly seen for the rows 40l and 30l where  $4028 < 4030$  and  $3037 \geq 3039$ . These discrepancies could neither be removed by small variations in the z parameters nor by assuming other distributions of the Ba atoms for the structure factor calculations. Other discrepancies found from Tables 1 and 2 are 222:224, 332:334, 0050:0052 and 1148:1152. However, for most reflexions the agreement is quite good and considering the errors which might be introduced by absorption effects and errors in the ratios  $f_M/f_{Bi}$  and  $f_0/f_{Bi}$  the agreement might on the whole be classified as fairly good.

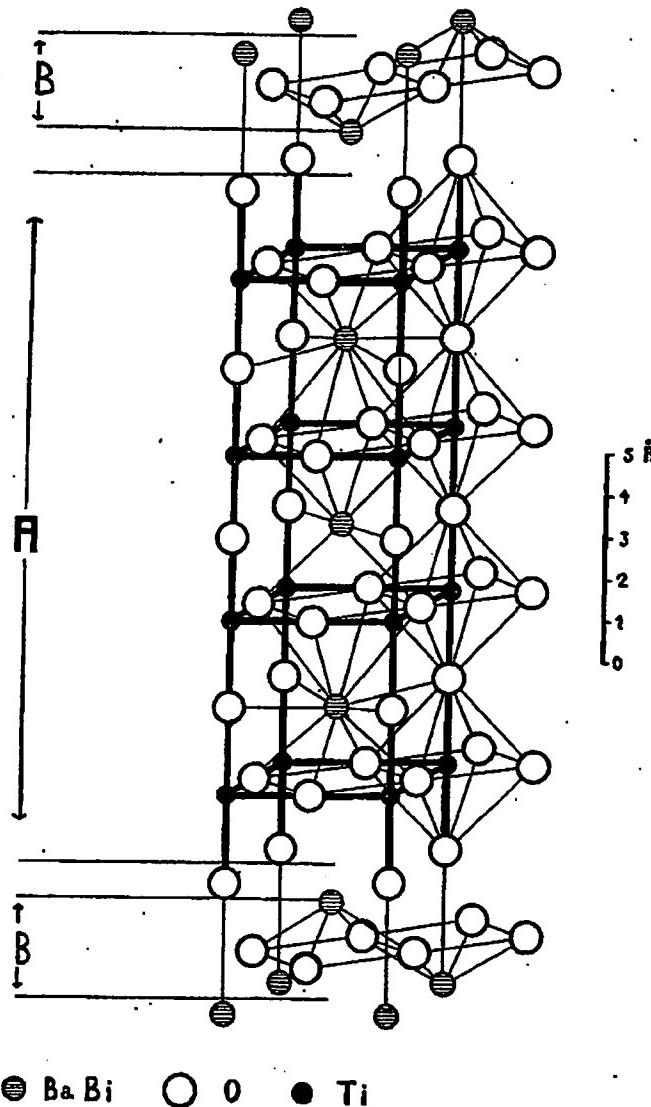
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Fig. 4. One half of the unit cell of  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$ . A denotes the perovskitic region and B the  $\text{Me}_2\text{O}_3$  layers.

The following structure is therefore proposed:  
 $D_{\bar{d}}^W - I4/mmm$   
 $(000, \frac{1}{2}\frac{1}{2}\frac{1}{2}) +$

- 2  $\text{Me}_1$  in 2 (a) 000
- 2  $\text{O}_1$  in 2 (b) 00 $\frac{1}{2}$
- 8  $\text{O}_2$  in 8 (g)  $0\frac{1}{2}z; 0\frac{1}{2}\bar{z}; \frac{1}{2}0z; \frac{1}{2}0\bar{z}$   $z = 0.048$
- 4  $\text{Ti}_1$  in 4 (e)  $00z; 00\bar{z}$   $z = 0.452$
- 4  $\text{O}_3$  in 4 (e)  $z = 0.402$

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4 Me <sub>2</sub> in 4 (e)	$z = 0.106$
8 O <sub>4</sub> in 8 (g)	$z = 0.148$
4 Ti <sub>2</sub> in 4 (e)	$z = 0.352$
4 O <sub>5</sub> in 4 (e)	$z = 0.302$
4 Me <sub>3</sub> in 4 (e)	$z = 0.221$
4 O <sub>6</sub> in 4 (d) 0 $\frac{1}{2}$ $\frac{1}{2}$ ; $\frac{1}{2}$ 0 $\frac{1}{2}$	

Ba and Bi equally distributed over all Me positions.

If the structure is described by means of an orthorhombic space group ( $D_{2h}^{22}$ ), as used for the structures of  $\text{Bi}_3\text{NbTiO}_9$  and  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$ , the positions will be:  $D_{2h}^{22}$  — F  $m m m$  (000;  $\frac{1}{2}\frac{1}{2}0$ ;  $0\frac{1}{2}\frac{1}{2}$ ;  $\frac{1}{2}0\frac{1}{2}$ ) + 4 Me<sub>1</sub> in 4 (a) 000, 4 O<sub>1</sub> in 4 (b) 00 $\frac{1}{2}$ , 16 O<sub>2</sub> in 16 (j)  $\frac{1}{2}\frac{1}{2}z$ ;  $\frac{1}{2}\frac{1}{2}\bar{z}$ ;  $\frac{1}{2}\frac{1}{2}z$ ;  $\frac{1}{2}\frac{1}{2}\bar{z}$ ;  $z = 0.048$ , 8 Ti<sub>1</sub> in 8 (i) 00z; 00 $\bar{z}$   $z = 0.452$ , 8 O<sub>3</sub> in 8 (i)  $z = 0.402$ , 8 Me<sub>2</sub> in 8 (i)  $z = 0.106$ , 16 O<sub>4</sub> in 16 (j)  $z = 0.148$ , 8 Ti<sub>2</sub> in 8 (i)  $z = 0.352$ , 8 O<sub>5</sub> in 8 (i)  $z = 0.302$ , 8 Me<sub>3</sub> in 8 (i)  $z = 0.221$ , 8 O<sub>6</sub> in 8 (f)  $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ ;  $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ .

The distances ( $\text{\AA}$ ) and coordination will be:

$O_1 - 8 O_2 = 2.78$	$O_2 - 4 O_3 = 2.73$	$Me_2 - 4 O_2 = 3.10$	$Ti_1 - O_3 = 2.09$
$O_3 - 4 O_2 = 2.84$	$O_4 - 4 O_4 = 2.73$	$Me_2 - 4 O_3 = 2.75$	$Ti_1 - 4 O_2 = 1.93$
$O_3 - 4 O_4 = 2.84$	$O_6 - 4 O_6 = 2.73$	$Me_2 - 4 O_4 = 2.61$	$Ti_1 - O_1 = 2.00$
$O_5 - 4 O_6 = 2.91$			
$Me_1 - 8 O_2 = 2.78$	$Me_3 - 4 O_6 = 2.28$	$Ti_2 - O_3 = 2.09$	
$Me_1 - 4 O_1 = 2.73$	$Me_3 - 4 O_5 = 2.89$	$Ti_3 - 4 O_4 = 1.93$	
	( $Me_3 - 4 O_4 = 3.64$ )	$Ti_3 - O_5 = 2.09$	

One half of the unit cell is shown in Fig. 4.

I wish to thank Professor L. G. SILLÉN for valuable discussions on this work.

Stockholms Högskola, Institute of Inorganic and Physical Chemistry. May 1950.

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Tryckt den 14 oktober 1950

Uppsala 1950. Almqvist & Wiksell's Boktryckeri AB

# **BRIEF ATTACHMENT Y**

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of

Applicants: Bednorz et al.

Serial No.: 08/479,810

Filed: June 7, 1995

For: NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION

Date: March 1, 2005

Docket: YO987-074BZ

Group Art Unit: 1751

Examiner: M. Kopeć

Commissioner for Patents

P.O. Box 1450

Alexandria, VA 22313-1450

**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT Y**

## ARKIV FÖR KEMI Band 5 nr 4

Communicated 14 May 1952 by ARNE WESTGREN

The structure of  $\text{Bi}_2\text{NbO}_5\text{F}$  and isomorphous compounds

By BENGT AURIVILLIUS

With 1 figure in the text

X-ray studies made previously on the compounds  $\text{CaBi}_2\text{Nb}_2\text{O}_9$ ,  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  and  $\text{BaBi}_4\text{Ti}_4\text{O}_{15}$  (1) showed that they have very similar structures. The symmetry is tetragonal or pseudotetragonal, and the structures are each built up of quadratic  $\text{Bi}_2\text{O}_3$  layers alternating with perovskite layers, the latter having different heights in the three different cases. The generalized formula for the compounds might be written  $Me_2\text{O}_2 (Me_{m-1} R_m \text{O}_{8m+1})$  where  $Me'$  is the 12 coordinated metal atom in the perovskite layers and  $R$  the 6 coordinated atom. The formulae for the above compounds,  $\text{Bi}_2\text{O}_2(\text{CaNb}_2\text{O}_7)$ ,  $\text{Bi}_2\text{O}_2(\text{Bi}_2\text{Ti}_3\text{O}_{10})$  and  $\text{Bi}_2\text{O}_2[(\text{BaBi}_2)\text{Ti}_4\text{O}_{15}]$  thus have  $m$  values of 2, 3 and 4. The simplest case,  $m=1$ , would correspond to the formula  $Me_2\text{O}_2(RO_6)$  and to a structure built up of  $Me_2\text{O}_2$  layers and layers of  $RO_6$  octahedra each octahedron sharing four corners. Compounds of this type have, however, not been successfully synthesized as yet.

The present paper deals with the compounds  $\text{Bi}_2\text{NbO}_5\text{F}$ ,  $\text{Bi}_2\text{TaO}_5\text{F}$  and  $\text{Bi}_2\text{TiO}_4\text{F}_2$ , which correspond to the simplest case,  $m=1$  above, except that some of the O atoms are replaced by F atoms. The formulae of the compounds might thus be written:  $\text{Bi}_2(O, F)_2\text{Nb}(O, F)_4$  etc.

## Preparation, powder photographs and analyses

$\text{Bi}_2\text{NbO}_5\text{F}$ : When a mixture of  $\text{BiF}_3$  and  $\text{Nb}_2\text{O}_5$  in the mol ratio 4:1 was heated in air at  $800^\circ\text{C}$  for a short time, a few single crystals (very thin plates) were obtained. Powder photographs of this sample indicated a tetragonal unit cell with the same cell dimensions as would be expected for the above general type when  $m=1$ . The best conditions for the formation of this phase were then studied by heating 2.5 g mixtures ( $2\text{BiF}_3 + \frac{1}{2}\text{Nb}_2\text{O}_5$ ) in air at  $640^\circ\text{C}$ , this low temperature being chosen to reduce the volatility of the  $\text{BiF}_3$ . The reaction times were varied from 5–40 hours, and powder photographs were taken of each product. For reaction times of 7–15 hours the lines of the above tetragonal phase predominated in the powder photographs, the few extra lines were very weak (see Table 1).

The fluorine content was found to vary from 4.0 % (7 hours) to 2.4 % (15 hours), whereas the calculated value for  $\text{Bi}_2\text{NbO}_5\text{F}$  is 3.2 %. No variation in the size of the cell with the fluorine content was found, and it therefore seems probable that the composition of the phase is constant and that the observed variation in the F content is due to the presence of small impurities which are not visible in the powder photo-

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*Table 1*  
 Powder photographs of  $\text{Bi}_2\text{NbO}_5\text{F}$  (sample with 2.8 % F)  
 $O\bar{r} K$  radiation  $\lambda_{O, K_a} = 2.2909 \text{ \AA}$

$h k l$	$10^4 \cdot \sin^2 \theta_{\text{calc}}$	$10^4 \cdot \sin^2 \theta_{\text{obs}}$	$I_{\text{obs}}$
1 0 3	1319	1332	st
0 0 6	1708	1711	m
1 1 0	1784	1795	m
1 1 2	1974	1969	vvv
1 0 5	2078	2083	vv
1 1 4	2543	2547	m
—	—	2785	vvv
0 0 8	3036	3033	w
—	—	3093	vw
1 1 6	3492	3490	st
2 0 0	3568	3567	st
2 0 2	3758	3754	vw
—	—	3808	vv
{ 1 0 9	4734 }	4737	st
{ 0 0 10	4743 }	4737	st
1 1 8	4820	4827	w
2 1 3	4888	4891	st
2 0 6	5278	5292	m
2 1 5	5647	5658	w
1 1 10	6527	6529	vw
1 0 11	6631	6630	w
0 0 12	6830	6841	w
2 2 0	7137	7139	w
2 2 2	7327	7330	vw
3 0 1	8076	8080	vvv
{ 2 1 9	8303 }	8304	st
{ 2 0 10	8311 }	8304	st
3 0 3	8456	8456	m
1 1 12	8614	8611	m
2 2 6	8845	8844	m
{ 1 0 13	8908 }	8919	m
3 1 0	8921	8919	m
3 1 2	9111	9119	vw
3 0 5	9215	9195	vw
0 0 14	9297	9292	vw

Fig. 1. C

$\text{Bi}_2\text{TiO}_5$   
 2:1 (total  
 photographs  
 assuming  
 the same  
 phase are  
 of the mi-  
 variation  
 are 7.8 %  
 fluorine a  
 of  $\text{Bi}_2\text{NbO}_5$   
 $\text{Bi}_2\text{TiO}_4\text{F}_2$

Method  
 with  $\text{NaOJ}$   
 (3). The di-

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graphs. To check that the Bi/Nb ratio had not changed essentially during the heating, a complete analysis was made on one sample (9 hours heating). The following values were obtained as the mean of three analyses: Bi:  $68.0 \pm 0.6\%$ , Nb:  $14.2 \pm 0.6\%$ , F:  $3.7 \pm 0.2\%$ .

The values calculated for  $\text{Bi}_2\text{NbO}_5\text{F}$  are:

Bi: 68.5%, Nb: 15.2%, F: 3.2%.

From these figures it seems probable that the formula of the compound is  $\text{Bi}_2\text{NbO}_5\text{F}$ .

$\text{Bi}_2\text{TaO}_5\text{F}$  was prepared in exactly the same way as  $\text{Bi}_2\text{NbO}_5\text{F}$ . No analysis was made since the powder photographs were similar to those of  $\text{Bi}_2\text{NbO}_5\text{F}$  and niobium and tantalum compounds are usually isomorphous.

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B)

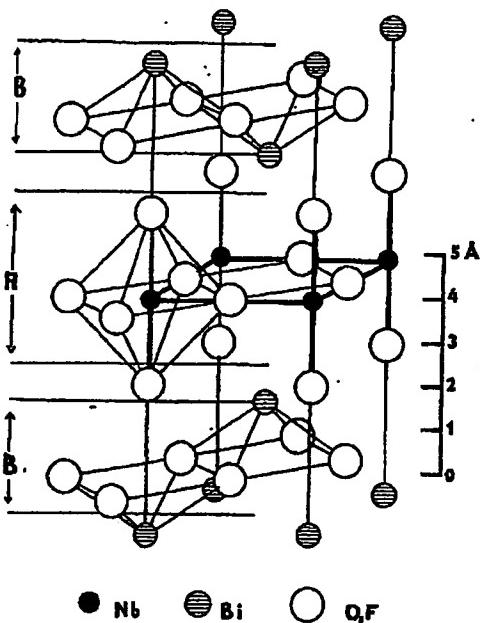


Fig. 1. One half of the unit cell of  $\text{Bi}_2\text{NbO}_5\text{F}$ . A denotes the region of  $\text{Nb}(\text{O},\text{F})_6$  octahedra and B the  $\text{Bi}_2(\text{O},\text{F})_3$  layers.

$\text{Bi}_2\text{TiO}_4\text{F}_3$ : Mixtures of bismuth fluoride and titanium oxide in the mol ratio 2:1 (total 2.3 g) were heated in air at  $640^\circ$  for various lengths of time. The powder photographs obtained from samples heated for 3 or 5 hours could be interpreted by assuming a mixture of  $\text{BiOF}$  (2) and a phase whose cell dimensions were nearly the same as those of  $\text{Bi}_2\text{NbO}_5\text{F}$ . (See Table 2, where the reflexions from the  $\text{BiOF}$  phase are designated by  $b$  and those from the other phase by  $a$ ). The fluorine contents of the mixed samples were found to be 6.4 % (5 hours) and 8.4 % (3 hours) but no variation of the cell size with the fluorine content was found. The calculated values are 7.8 % for  $\text{BiOF}$  and 6.7 % for  $\text{Bi}_2\text{TiO}_4\text{F}_3$ . From the original  $\text{Bi}/\text{Ti}$  ratio, from the fluorine analysis and from the similarity of the powder photographs with those of  $\text{Bi}_2\text{NbO}_5\text{F}$  (Tables 1 and 2), it was concluded that the formula of the phase is  $\text{Bi}_2\text{TiO}_4\text{F}_3$ .

the heating, owing values  
 $2 \pm 0.6\%$ , F:

Methods of analysis: Fluorine. The samples were first decomposed by fusing with  $\text{NaOH}$ , and were then distilled with  $\text{HClO}_4$  as described by WILLARD and WINTER (3). The distillate was titrated with  $\text{Th}(\text{NO}_3)_4$  using Na-alizarinsulphonate as indicator.

Bismuth and Niobium. The samples were brought into solution, and niobium was determined as described in Scott's "Standard Methods" (4). Bismuth was first precipitated as  $\text{Bi}_2\text{S}_3$ , which was then redissolved, converted to  $\text{Bi}_2\text{O}_3$  and weighed as such.

s  $\text{Bi}_2\text{NbO}_5\text{F}$ .

No analysis  
 $\text{NbO}_5\text{F}$  and

#### Unit cells and space group

The dimensions of the unit cells were determined from powder photographs taken with focusing cameras of the Phragmén type (Tables 1 and 2). The radiation used

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Table 2

Powder photographs of  $\text{Bi}_2\text{TiO}_4\text{F}_2$  (mixed with  $\text{BiOF}$ )  $\text{CrK}$  radiation ( $\lambda_{\text{CrK}\alpha} = 2.2909 \text{ \AA}$ ).  $a$  denotes the  $\text{Bi}_2\text{TiO}_4\text{F}_2$  phase and  $b$  the  $\text{BiOF}$  phase

$hkl$	phase	$10^4 \sin^2 \theta_{\text{calc}}$	$10^4 \sin^2 \theta_{\text{obs}}$	$I_{\text{obs}}$
1 0 1	$a$	957	941	vvv
1 0 1	$b$	1270	1265	m
{ 1 0 3	$a$	1351 }		
{ 0 0 2	$b$	1352 }	1354	st
0 0 6	$a$	1771	1767	m
1 1 0	$a$	1816	1811	m
1 1 0	$b$	1864	1858	vvv
1 1 2	$a$	2013	1999	w
1 0 5	$a$	2138	2132	w+
1 0 2	$b$	2284	2288	vvv
1 1 4	$a$	2603	2601	m
-	-	-	3074	vv
1 1 2	$b$	3216	3231	w
1 0 7	$a$	3319	3320	vv
1 1 6	$a$	3587	3600	st
2 0 0	$a$	3631	3624	st
2 0 0	$b$	3728	3744	w
2 0 2	$a$	3828	3822	w
1 0 3	$b$	3974	3982	w
-	-	-	4352	vvv
2 0 4	$a$	4418	4426	vvv
2 1 1	$a$	4598	4590	w
-	-	-	4674	vvv
{ 1 0 9	$a$	4893 }		
{ 1 1 3	$b$	4906 }	4904	st
{ 0 0 10	$a$	4919 }		
2 1 3	$a$	4982	4979	st
2 0 2	$b$	5080	5084	w
{ 2 0 6	$a$	5402 }		
{ 0 0 4	$b$	5408 }	5416	m+
2 1 5	$a$	5769	5788	m
2 1 2	$b$	6012	6025	m
1 0 4	$b$	6340	6353	w
{ 2 0 3	$b$	6770 }		
{ 2 0 8	$a$	6779 }	6786	m
1 0 11	$a$	6860	6869	m
2 1 7	$a$	6950	6950	vvv
0 0 12	$a$	7084	7075	m
{ 2 2 0	$a$	7262 }		
{ 1 1 4	$b$	7272 }	7262	m
{ 2 2 0	$b$	7455 }		
{ 2 2 2	$a$	7459 }	7456	w
2 1 3	$b$	7702	7709	m
-	-	-	8049	vv
3 0 1	$a$	8210	8210	vv
-	-	-	8352	vv
{ 2 1 9	$a$	8524 }		
{ 2 0 10	$a$	8550 }	8524	st
3 0 3	$a$	8613	8603	m
3 0 1	$b$	8736	8725	w
2 2 2	$b$	8814	8807	w
1 1 12	$a$	8900	8900	m

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radiation  
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Table 2 (continued)

<i>h k l</i>	phase	$10^4 \sin^2 \theta_{\text{calc}}$	$10^4 \sin^2 \theta_{\text{obs}}$	$I_{\text{obs}}$
2 2 6	<i>a</i>	9033	9027	
3 1 0	<i>a</i>	9078	9072	w
2 0 4	<i>b</i>	9136	9186	vw
3 1 2	<i>a</i>	9275	9272	m
3 1 0	<i>b</i>	9319	9319	w
{ 1 0 5	<i>b</i>	9382 }	9384	
{ 3 0 5	<i>a</i>	9400 }		m

was  $\text{Cr } K$  ( $\lambda_{\text{Cr } K} = 2.2909 \text{ \AA}$ ). As mentioned above the powder photographs could be interpreted by assuming tetragonal unit cells; the cell dimensions are given below.

	<i>a</i> (\text{\AA})	<i>c</i> (\text{\AA})
$\text{Bi}_2\text{NbO}_5\text{F}$ .....	3.835	16.63
$\text{Bi}_2\text{TaO}_5\text{F}$ .....	3.829	16.64
$\text{Bi}_2\text{TiO}_4\text{F}_2$ .....	3.802	16.33

The errors in these figures are estimated to be  $\pm 0.1\%$ .

The observed density was 8.0 for  $\text{Bi}_2\text{NbO}_5\text{F}$  (preparation with 2.8% F), which agrees fairly well with the assumption of 2 formula units per unit cell, giving a calculated density of 8.26.

Zero and first order Weissenberg photographs around the *a* axis were taken. There was nothing in the Weissenberg photographs to indicate a Laue symmetry lower than  $D_{4h}$ —4/mmm. The only extinctions found were that *h*, *k*, *l* were absent for *h+k+l* odd, which is characteristic of the space groups  $C_{4v}^0$ ,  $D_{2d}^0$ ,  $D_{2d}^{11}$  and  $D_{4h}^{17}$ .

Powder photographs only were taken of the compounds  $\text{Bi}_2\text{TaO}_5\text{F}$  and  $\text{Bi}_2\text{TiO}_4\text{F}_2$ , and from these it was concluded that these substances are isomorphous with  $\text{Bi}_2\text{NbO}_5\text{F}$ .

#### Positions of the metal atoms

$\text{Bi}_2\text{NbO}_5\text{F}$ : With 2 formula units per unit cell there are 4 Bi and 2 Nb atoms per unit cell. The intensities of the spots in the Weissenberg photographs seemed in the main to depend only on the *l* values. Thus for *l* even  $I_{00l} \approx I_{11l} \approx I_{20l}$ , etc. and for *l* odd:  $I_{10l} \approx I_{11l} \approx I_{20l}$ , etc. With these intensity values a good approximation of the Patterson-Harker function along 00*z* could be obtained by using only the intensity values of  $h0l$  and  $h1l$ . The Patterson-Harker function thus calculated (not given here) showed only one, big, maximum, at *z*=0.34. This maximum, and the absence of others, could be explained only by assuming that 4 Bi atoms are situated at the positions  $\pm 00z$  with *z*=0.17 or *z*=0.33, and the Nb atoms at the positions  $00\frac{1}{2}$  or  $000$ . Arbitrarily choosing  $000$  as the position for Nb, trial and error calculations gave the value 0.325 for the Bi parameter.

No determination of  $z_{\text{Bi}}$  was made for  $\text{Bi}_2\text{TaO}_5\text{F}$ .

For  $\text{Bi}_2\text{TiO}_4\text{F}_2$  the powder photograph data were used to determine the Bi parameter. Assuming the Ti atoms to be situated at  $000$  and the O and the F atoms to occupy the same positions as given below for  $\text{Bi}_2\text{NbO}_5\text{F}$ , the value  $z_{\text{Bi}}=0.327 \pm 0.006$  was obtained from trial and error calculations.

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Table 3  
Weissenberg photographs of  
 $\text{Bi}_2\text{NbO}_5\text{F}$

Zero layer

$l$	$h k$	0 0		2 0		4 0		$l$
		$I_{\text{calo}}$	$I_{\text{obs}}$	$I_{\text{calo}}$	$I_{\text{obs}}$	$I_{\text{calo}}$	$I_{\text{obs}}$	
0		—	—	170	vst	37	w	0
2		—	—	10	w	3	vw	2
4		0.3	—	0.04	—	0.05	—	4
6		220	vst	67	w	34	vw	6
8		12	w	5	vw	6	vvw	8
10		3	vw	2	—	2	—	10
12		44	st	26	w	86	st	12
14		15	m	11	w			14
16		10	w	10	w			16
18		16	m	28	m			18
20		22	m					20
$l$	$h k$	1 0		3 0		$l$		$l$
		$I_{\text{calo}}$	$I_{\text{obs}}$	$I_{\text{calo}}$	$I_{\text{obs}}$			
1		7	w	1	vw	1		1
3		270	vst	42	w	3		3
5		40	w	8	vw	5		5
7		1	—	0.2	—	7		7
9		75	m	30	vw			9
11		18	w	10	vw			11
13		3	vw	3	vw			13
15		20	m	19	m			15
17		12	w					17
19		14	w					19

## Positions of the O and the F atoms

The positions of the O and the F atoms could not be distinguished either from the diffraction data, or from space considerations because of the similarity in the reflecting power and ionic radii of  $\text{O}^{2-}$  and  $\text{F}^-$ . The problem is therefore treated as though O and F were the same atomic species. In the following, the O and the F atoms are denoted by (O, F) and the discussion relates to  $\text{Bi}_2\text{NbO}_5\text{F}$  for which  $z_{\text{Bi}}$  could be accurately determined from the Weissenberg photographs.

It seemed reasonable to assume that the Nb atoms are surrounded by a regular or nearly regular octahedron of (O, F) atoms with distances  $\text{Nb}-(\text{O}, \text{F}) \approx 2.0 \text{ \AA}$ . Neglecting the polar space group  $C_{4v}^h$ , these conditions are fulfilled only if 4 (O, F) atoms, here called  $(\text{O}, \text{F})_1$ , are situated at the positions  $\pm 00z$  with  $z \approx 0.12$ , and 4 (O, F) atoms,  $(\text{O}, \text{F})_2$ , at the positions  $0\frac{1}{2}0, \frac{1}{2}00$ . Assuming the distance  $(\text{O}, \text{F})-(\text{O}, \text{F})$  to be  $\geq 2.5 \text{ \AA}$  and the distance  $\text{Bi}-(\text{O}, \text{F})$  to be  $\geq 2.2 \text{ \AA}$  there is only room for the remaining 4 (O, F) atoms,  $(\text{O}, \text{F})_3$ , at the positions  $0\frac{1}{2}\frac{1}{2}, \frac{1}{2}0\frac{1}{2}$ .

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Table  
photographs of  $\text{NbO}_6\text{F}$   $\text{Cu K}\alpha$  radiation

## First layer

4 0		$h k$	1 1		3 1	
$I_{\text{calc}}$	$I_{\text{obs}}$	1	$I_{\text{calc}}$	$I_{\text{obs}}$	$I_{\text{calc}}$	$I_{\text{obs}}$
37	w	0	210	vst	36	w
3	vv	2	17	w	4	vvv
0.05	—	4	11	w	2	—
34	vw	6	110	m	33	w
6	vvv	8	27	vw	9	vw
.....		.....				
2	—	10	2	vvw	1	—
		12	21	m	20	w
86	st	14	14	w	20	w
		16	5	w	17	w
		18	19	m		
		20	58	st		
4 1		$h k$	0 1		2 1	
		1	$I_{\text{calc}}$	$I_{\text{obs}}$	$I_{\text{calc}}$	$I_{\text{obs}}$
		1	7	—	2	vw
		3	270	vst	74	m
		5	40	m	13	w
		7	1	—	0.3	—
		9	75	vst	40	w
		11	18	m	12	vvw
		13	8	vw	3	vw
		15	20	m	19	m
		17	12	w	19	m
		19	14	w		

The coordination and distances in Å will be:

$$\text{Bi}-4(\text{O}, \text{F})_3 = 2.29 \quad \text{Nb}-2(\text{O}, \text{F})_1 = 2.0$$

$$\text{Bi}-4(\text{O}, \text{F})_1 = 2.9 \quad \text{Nb}-4(\text{O}, \text{F})_2 = 1.92$$

$$(\text{O}, \text{F})_3-4(\text{O}, \text{F})_3 = 2.71 \quad (\text{O}, \text{F})_2-4(\text{O}, \text{F})_2 = 2.71$$

$$(\text{O}, \text{F})_1-4(\text{O}, \text{F})_3 = 2.9 \quad (\text{O}, \text{F})_1-4(\text{O}, \text{F})_2 = 2.8$$

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 $(\text{O}, \text{F}) \approx 2.0 \text{ \AA}$   
only if  $4(\text{O}, \text{F})$   
th  $z \approx 0.12$ , and  
distance  $(\text{O}, \text{F})$ —  
is only room for

The proposed structure is given in the summary. Calculated and observed intensities for the reflexions in the Weissenberg photographs are given in Table 3.  $I_{\text{calc}}$  is derived as follows:

$$I_{\text{calc}} = \frac{1 + \cos^2 2\theta}{1600 \cdot \sin 2\theta} \cdot F^2 \text{ where } F = \sum f \cos 2\pi(hx + ky + lz).$$

The lines of maximum absorption in the Weissenberg photographs (see 5) are indicated by dotted lines in Table 3. If the absorption effects are taken into account, the agreement between calculated and observed intensities is quite good.

**B. AURIVILLIUS, The structure of  $\text{Bi}_2\text{NbO}_5\text{F}$  and isomorphous compounds****Discussion of the structure**

Even if the  $(\text{O}, \text{F})_1$  atoms (see above) are assumed to occupy such a position that the distance  $\text{Bi}-4(\text{O}, \text{F})_1$  is as small as possible [ $z(\text{O}, \text{F})_1 = 0.15$ ,  $(\text{O}, \text{F})_1 - (\text{O}, \text{F})_3 = 2.5$ ,  $\text{Nb}-2(\text{O}, \text{F})_1 = 2.5$ ,  $\text{Bi}-4(\text{O}, \text{F})_1 = 2.7$ ], the distance  $\text{Bi}-4(\text{O}, \text{F})_1$  will still be much longer than the distance  $\text{Bi}-4(\text{O}, \text{F})_3$ . It therefore seems appropriate to describe the structure of  $\text{Bi}_2\text{NbO}_5\text{F}$  as being built up of  $\text{Bi}_2(\text{O}, \text{F})_2$  layers alternating with octahedral layers having the composition  $\text{Nb}(\text{O}, \text{F})_4$ , both layers being perpendicular to the  $c$ -axis. It might be pointed out that the structure of  $\text{Bi}_2(\text{O}, \text{F})_2\text{Nb}(\text{O}, \text{F})_4$  is basically of the same type as the " $X_1$  structures",  $M\text{e}_2\text{O}_3X$ , previously investigated by SILLÉN (6). Thus the octahedral sheets  $\text{Nb}(\text{O}, \text{F})_4$  correspond to single layers of halogen atoms,  $X$ , in  $M\text{e}_2\text{O}_3X$ .

**Discussion of the distribution of the O and the F atoms**

As seen above, the distance  $\text{Bi}-4(\text{O}, \text{F})_3$  is 2.29 Å for  $\text{Bi}_2\text{NbO}_5\text{F}$ . For  $\text{Bi}_2\text{TiO}_4\text{F}$ , the corresponding distance is calculated to be  $2.26 \pm 0.06$  Å. These distances are very nearly the same as the corresponding distances,  $\text{Bi}-4(\text{O})$ , within the  $\text{Bi}_2\text{O}_3$  layers of other bismuth oxides (6). This need not, however, necessarily mean that the  $\text{Bi}_2(\text{O}, \text{F})_2$  layers (see the figure) are free from F atoms, since compounds with  $\text{Bi}_2(\text{O}, \text{F})_2$  layers which certainly contain F atoms have not been investigated hitherto, and thus the distances within such layers are unknown.

For the present it seems therefore best to make no special assumptions as to the distribution of the O and F atoms.

**SUMMARY**

The crystal structure of  $\text{Bi}_2\text{NbO}_5\text{F}$  has been investigated by means of Weissenberg and powder photographs. From powder photographs the compounds  $\text{Bi}_2\text{TaO}_5\text{F}$  and  $\text{Bi}_2\text{TiO}_4\text{F}_2$  have been found to be isomorphous with  $\text{Bi}_2\text{NbO}_5\text{F}$ . The following structure is proposed for  $\text{Bi}_2\text{NbO}_5\text{F}$ :

$D_{4h}^{17}-I\bar{4}/mmm$

$(0\ 0\ 0, \frac{1}{2}\frac{1}{2}\frac{1}{2})$	$+$	
2 Nb	in 2 (a)	: 0 0 0
4 Bi	in 4 (e)	: $\pm 0 0 z$
4 ( $\text{O}, \text{F}$ ) <sub>1</sub>	in 4 (c)	: $0 \frac{1}{2} 0, \frac{1}{2} 0 0$
4 ( $\text{O}, \text{F}$ ) <sub>2</sub>	in 4 (e)	: $\pm 0 0 z$
4 ( $\text{O}, \text{F}$ ) <sub>3</sub>	in 4 (d)	: $0 \frac{1}{2} \frac{1}{2}, \frac{1}{2} 0 \frac{1}{2}$

$$z = 0.325 \pm 0.001$$

$$z = 0.12 \pm 0.01$$

The cell dimensions are  $a = 3.835$  Å,  $c = 16.63$  Å for  $\text{Bi}_2\text{NbO}_5\text{F}$ . The positions of the metal atoms were determined from the diffraction data, those of the  $(\text{O}, \text{F})$  atoms from space considerations. Although it does not seem improbable that O atoms alone occupy the positions  $0 \frac{1}{2} \frac{1}{2}, \frac{1}{2} 0 \frac{1}{2}$ , Bi and O thus forming  $\text{Bi}_2\text{O}_3$  layers as in other bismuth oxides, nothing can be definitely stated as to the distribution of the O and F atoms.

The structure is built up of quadratic  $\text{Bi}_2(\text{O}, \text{F})_2$  layers alternating with octahedral sheets having the composition  $\text{Nb}(\text{O}, \text{F})_4$  (see figure) and the formula might thus be written:  $\text{Bi}_2(\text{O}, \text{F})_2\text{Nb}(\text{O}, \text{F})_4$ . The structure is formally related to a series of

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previously investigated structures of general formula  $M_{2m}O_3$  ( $M_{2m-1}R_mO_{3m+1}$ ) and represents the simplest case of this series, i.e.  $m=1$ .

such a position  
 $=0.15$ ,  $(O, F)_1$   
 $Bi-4 (O, F)_1$  will  
 before seems ap-  
 prop of  $Bi_2(O, F)_4$   
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 $(O, F)_4$  correspond

University of Stockholm, Institute of Inorganic and Physical Chemistry, May 1952.

REFERENCES. 1. Aurivillius, B., Arkiv Kemi 2 (1950) 519. — 2. —, Arkiv Kemi Mineral. Geol., 26 B (1948) no 2. — 3. Willard, H. H. and Winter, O. B., Ind. Eng. Chem. Anal. Ed. 5 (1933) 7. — 4. Standard Methods of Chemical Analysis by W. W. Scott, fifth edition, edited by N. H. Furman, New York 1925, p. 335 and p. 338. — 5. Wells, A. F., Z. Krist. 96 (1937) 451. — 6. Sillén, L. G., Dissert. Stockholm 1940.

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For  $Bi_2TiO_4F$ ,  
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**BRIEF ATTACHMENT Z**

**IN THE UNITED STATES PATENT AND TRADEMARK OFFICE**

In re Patent Application of

Applicants: Bednorz et al.

Serial No.: 08/479,810

Filed: June 7, 1995

For: NEW SUPERCONDUCTIVE COMPOUNDS HAVING HIGH TRANSITION  
TEMPERATURE, METHODS FOR THEIR USE AND PREPARATION

Date: March 1, 2005

Docket: YO987-074BZ

Group Art Unit: 1751

Examiner: M. Kopeć

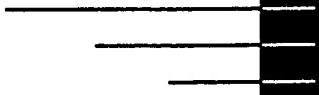
Commissioner for Patents  
P.O. Box 1450  
Alexandria, VA 22313-1450

**FIRST SUPPLEMENTAL AMENDMENT**

Sir:

In response to the Office Action dated July 28, 2004, please consider the  
following:

**ATTACHMENT Z**



# *Superconductivity*

*Charles P. Poole, Jr.*  
*Horacio A. Farach*  
*Richard J. Creswick*

Department of Physics and Astronomy  
University of South Carolina  
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# *Perovskite and Cuprate Crystallographic Structures*

## I. INTRODUCTION

Chapter 3 shows that the majority of single-element crystals have highly symmetrical structures, generally fcc or bcc, in which their physical properties are the same along the three crystallographic directions  $x$ ,  $y$ , and  $z$ . The NaCl-type and  $A1_5$  compounds are also cubic. Some compounds do have lower symmetries, showing that superconductivity is compatible with many different types of crystallographic structure, but higher symmetries are certainly more common. In this chapter we will describe the structures of the high-temperature superconductors, almost all of which are tetragonal or orthorhombic.

In Chapter 3, we also gave some examples of the role played by structure in determining the properties of superconductors. The highest transition tempera-

tures in alloys of transition metals are at the boundaries of instability between the bcc and hcp forms. The NaCl-type compounds have ordered vacancies on one or another lattice site. The magnetic and superconducting properties of the Chevrel phases depend on whether the large magnetic cations (i.e., positive ions) occupy eightfold sites surrounded by chalcogenide ions or whether the small magnetic ions occupy octahedral sites surrounded by Mo ions.

The structures described here are held together by electrons that form ionic or covalent bonds between the atoms. No account is taken of the conduction electrons, which are delocalized over the copper oxide planes and form Cooper pairs responsible for the superconducting properties below  $T_c$ . The following chapter will be devoted to explaining the role of these

conduction electrons within the frameworks of the Hubbard model and band theory. Whereas the present chapter describes atom positions in coordinate space, the following chapter relies on a reciprocal lattice elucidation of these same materials.

We begin with a description of perovskite and explain some reasons that perovskite undergoes various types of distortions. This prototype exhibits a number of characteristics that are common to the high-temperature superconducting cuprates (see Section V). We will emphasize the structural commonalities of these materials and make frequent comparisons between them. Our earlier work (Poole *et al.*, 1988) and the comprehensive review by Yvon and François (1989) may be consulted for more structural detail on the atom positions, interatomic spacings, site

and thallium high temperature superconductors (Medvedeva *et al.*, 1993).

We assume that all samples are well made and safely stored. Humidity can affect composition, and Garland (1988) found that storage of  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  in 98% humidity exponentially decreased the diamagnetic susceptibility with a time constant of 22 days.

## II. PEROVSKITES

Much has been written about the high-temperature superconductors being perovskite types, so we will begin by describing the structure of perovskites. The prototype compound barium titanate,  $\text{BaTiO}_3$ , exists in three crystallographic forms with the following lattice constants and unit cell volumes (Wyckoff, 1964):

cubic:	$a = b = c = 4.0118 \text{ \AA}$	$V = 64.57 \text{ \AA}^3$
tetragonal:	$a = b = 3.9947, c = 4.0336$	$V = 64.37 \text{ \AA}^3$
orthorhombic:	$a = 4.009\sqrt{2} \text{ \AA}, b = 4.018\sqrt{2} \text{ \AA}, c = 3.990 \text{ \AA}$	$V = 2(64.26) \text{ \AA}^3$

symmetries, etc., of these compounds. There have been reports of superconductivity in certain other cuprate structures (e.g., Murphy *et al.*, 1987), but these will not be reported on in this chapter.

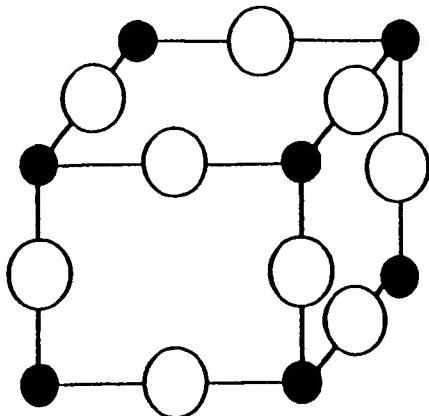
There is a related series of layered compounds  $\text{Bi}_2\text{O}_2(M_{m-1}R_m\text{O}_{3m+1})$  called Aurivillius (1950, 1951, 1952) phases, with the 12-coordinated  $M = \text{Ca}, \text{Sr}, \text{Ba}, \text{Bi}, \text{Pb}, \text{Cd}, \text{La}, \text{Sm}, \text{Sc}$ , etc., and the 6-coordinated transition metal  $R = \text{Nb}, \text{Ti}, \text{Ta}, \text{W}, \text{Fe}$ , etc. The  $m = 1$  compound  $\text{Bi}_2\text{NbO}_6$  belongs to the same tetragonal space group  $I4/mmm, D_{4h}^{17}$  as the lanthanum, bismuth,

For all three cases the crystallographic axes are mutually perpendicular. We will comment on each case in turn.

### A. Cubic Form

Above 201°C barium titanate is cubic and the unit cell contains one formula unit  $\text{BaTiO}_3$  with a titanium atom on each apex, a barium atom in the body center, and an oxygen atom on the center of each edge of the cube, as illustrated in Fig. 7.1. This corresponds to the barium atom, titanium atom, and three oxygen atoms being placed in positions with the following  $x, y$ , and  $z$  coordinates:

E site: Ti	$(0, 0, 0)$	Ti on apex
F site: O	$(0, 0, \frac{1}{2}); (0, \frac{1}{2}, 0); (\frac{1}{2}, 0, 0)$	three oxygens centered on edges
C site: Ba	$(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	Ba in center.



**Figure 7.1** Barium titanate ( $\text{BaTiO}_3$ ) perovskite cubic unit cell showing titanium (small black circles) at the vertices and oxygen (large white circles) at the edge-centered positions. Ba, not shown, is at the body center position (Poole *et al.*, 1988, p. 73).

The barium in the center has 12 nearest-neighbor oxygens, so we say that it is 12-fold coordinated, while the titanium on each apex has 6-fold (octahedral) coordination with the oxygens, as may be seen from the figure. (The notation *E* for edge, *F* for face, and *C* for center is adopted for reasons that will become clear in the discussion which follows.) Throughout this chapter we will assume that the *z*-axis is oriented vertically, so that the *x* and *y* axes lie in the horizontal plane.

Ordinarily, solid-state physics texts place the origin (0,0,0) of the perovskite unit cell at the barium site, with titanium in the center and the oxygens at the centers of the cube faces. Our choice of origin facilitates comparison with the structures of the oxide superconductors.

This structure is best understood in terms of the sizes of the atoms involved. The ionic radii of  $\text{O}^{2-}$  (1.32 Å) and  $\text{Ba}^{2+}$  (1.34 Å) are almost the same, as indicated in Table 7.1, and together they form a perfect fcc lattice with the smaller  $\text{Ti}^{4+}$  ions (0.68 Å) located in octahedral holes surrounded entirely by oxygens. The octahedral holes of a close-packed oxygen lattice have a radius of 0.545 Å; if these holes were empty the lattice constant would be  $a = 3.73$  Å, as noted in Fig. 7.2a. Each

titanium pushes the surrounding oxygens outward, as shown in Fig. 7.2b, thereby increasing the lattice constant. When the titanium is replaced by a larger atom, the lattice constant expands further, as indicated by the data in the last column of Table 7.2. When Ba is replaced by the smaller Ca (0.99 Å) and Sr (1.12 Å) ions, by contrast, there is a corresponding decrease in the lattice constant, as indicated by the data in columns 3 and 4, respectively, of Table 7.2. All three alkaline earths, Ca, Sr, and Ba, appear prominently in the structures of 3 high-temperature superconductors.

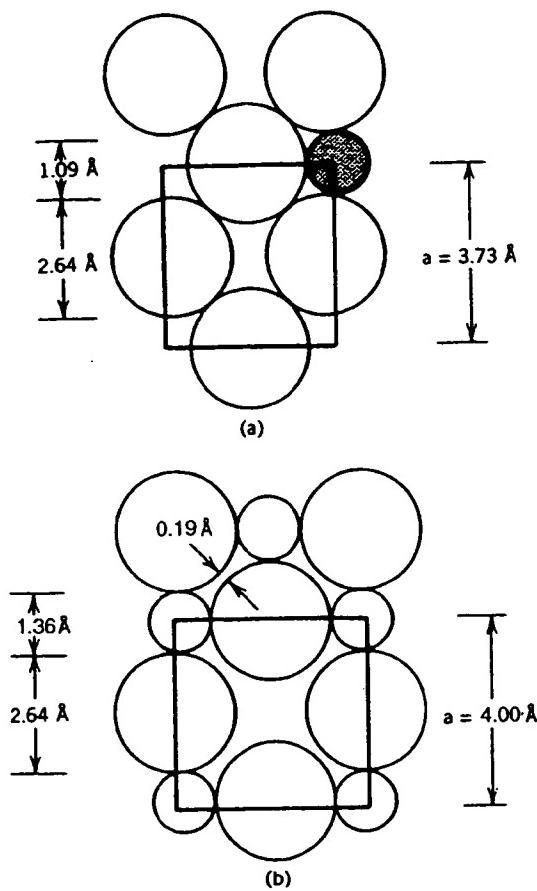
## B. Tetragonal Form

At room temperature barium titanate is tetragonal and the deviation from cubic,  $(c - a)/\frac{1}{2}(c + a)$ , is about 1%. All of the atoms have the same *x*, *y* coordinates as in the cubic case, but are shifted along the *z*-axis relative to each other by  $\approx 0.1$  Å, producing the puckered arrangement shown in Fig. 7.3. The distortions from the ideal structure are exaggerated in this sketch. The puckering bends the Ti-O-Ti group so that the Ti-O distance increases while the Ti-Ti distance remains almost

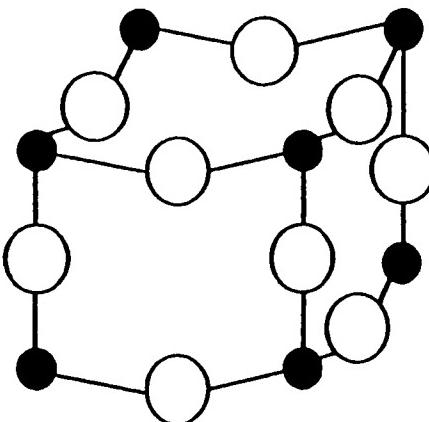
**Table 7.1** Ionic Radii for Selected Elements<sup>a</sup>

Small	$\text{Cu}^{2+}$	0.72 Å	$\text{Bi}^{5+}$	0.74 Å
Small-	$\text{Cu}^+$	0.96 Å	$\text{Y}^{3+}$	0.94 Å
Medium	$\text{Bi}^{3+}$	0.96 Å	$\text{Ti}^{3+}$	0.95 Å
	$\text{Ca}^{2+}$	0.99 Å	$\text{Bi}^{3+}$	0.96 Å
	$\text{Nd}^{3+}$	0.995 Å		
Medium-	$\text{Hg}^{2+}$	1.10 Å		
Large	$\text{Sr}^{2+}$	1.12 Å	$\text{La}^{3+}$	1.14 Å
	$\text{Pb}^{2+}$	1.20 Å	$\text{Ag}^+$	1.26 Å
Large	$\text{K}^+$	1.33 Å	$\text{O}^{2-}$	1.32 Å
	$\text{Ba}^{2+}$	1.34 Å	$\text{F}^-$	1.33 Å

<sup>a</sup> See Table VI-2 of Poole *et al.* (1988) for a more extensive list.



**Figure 7.2** Cross section of the perovskite unit cell in the  $z = 0$  plane showing (a) the size of the octahedral hole (shaded) between oxygens (large circles), and (b) oxygens pushed apart by the transition ions (small circles) in the hole sites. For each case the lattice constant is indicated on the right and the oxygen and hole sizes on the left (Poole *et al.*, 1988, p. 77).



**Figure 7.3** Perovskite tetragonal unit cell showing puckering of Ti–O layers that are perfectly flat in the cubic cell of Fig. 7.1. The notation of Fig. 7.1 is used (Poole *et al.*, 1988, p. 75).

the same. This has the effect of providing more room for the titanium atoms to fit in their lattice sites. We will see later that a similar puckering distortion occurs in the high-temperature superconductors as a way of providing space for the Cu atoms in the planes.

### C. Orthorhombic Form

There are two principal ways in which a tetragonal structure distorts to form an orthorhombic phase. The first, shown at

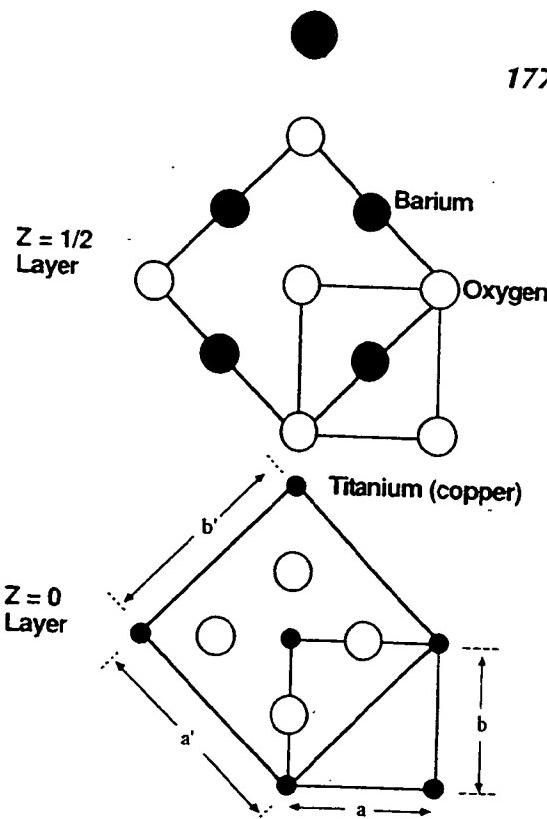
**Table 7.2** Dependence of Lattice Constants  $a$  of Selected Perovskites  $AMO_3$  on Alkaline Earth  $A$  and Ionic Radius of Transition Metal Ion  $M^{+4}$ ; the Alkaline Earth Ionic Radii are  $0.99 \text{ \AA}$  (Ca),  $1.12 \text{ \AA}$  (Sr), and  $1.34 \text{ \AA}$  (Ba)<sup>a</sup>

Transitional metal	Transitional metal radius, $\text{\AA}$	Lattice constant $a$ , $\text{\AA}$		
		Ca	Sr	Ba
Ti	0.68	3.84	3.91	4.01
Fe	—	—	3.87	4.01
Mo	0.70	—	3.98	4.04
Sn	0.71	3.92	4.03	4.12
Zr	0.79	4.02	4.10	4.19
Pb	0.84	—	—	4.27
Ce	0.94	3.85	4.27	4.40
Th	1.02	4.37	4.42	4.80

<sup>a</sup> Data from Wyckoff (1964, pp. 391ff).

the top of Fig. 7.4, is for the  $b$ -axis to stretch relative to the  $a$ -axis, resulting in the formation of a rectangle. The second, shown at the bottom of the figure, is for one diagonal of the  $ab$  square to stretch and the other diagonal to compress, resulting in the formation of a rhombus. The two diagonals are perpendicular, rotated by  $45^\circ$  relative to the original axes, and become the  $a'$ ,  $b'$  dimensions of the new orthorhombic unit cell, as shown in Fig. 7.5. These  $a'$ ,  $b'$  lattice constants are  $\approx \sqrt{2}$  times longer than the original constants, so that the volume of the unit cell roughly doubles; thus, it contains exactly twice as many atoms. (The same  $\sqrt{2}$  factor appears in Eq. 7.1 in our discussion of the lattice constants for the orthorhombic form of barium titanate.)

When barium titanate is cooled below  $5^\circ\text{C}$  it undergoes a diagonal- or rhombal-type distortion. The atoms have the same  $z$  coordinates ( $z = 0$  or  $\frac{1}{2}$ ) as in the cubic phase, so the distortion occurs entirely in the  $x$ ,  $y$ -plane, with no puckering of the atoms. The deviation from tetragonality, as



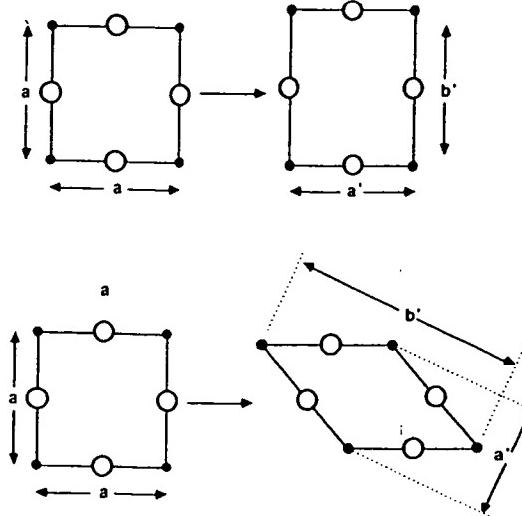
**Figure 7.5** Rhombal expansion of monomolecular tetragonal unit cell (small squares, lower right) to bimolecular orthorhombic unit cell (large squares) with new axes  $45^\circ$  relative to the old axes. The atom positions are shown for the  $z = 0$  and  $z = \frac{1}{2}$  layers (Poole *et al.*, 1988, p. 76).

given by the percentage of anisotropy,

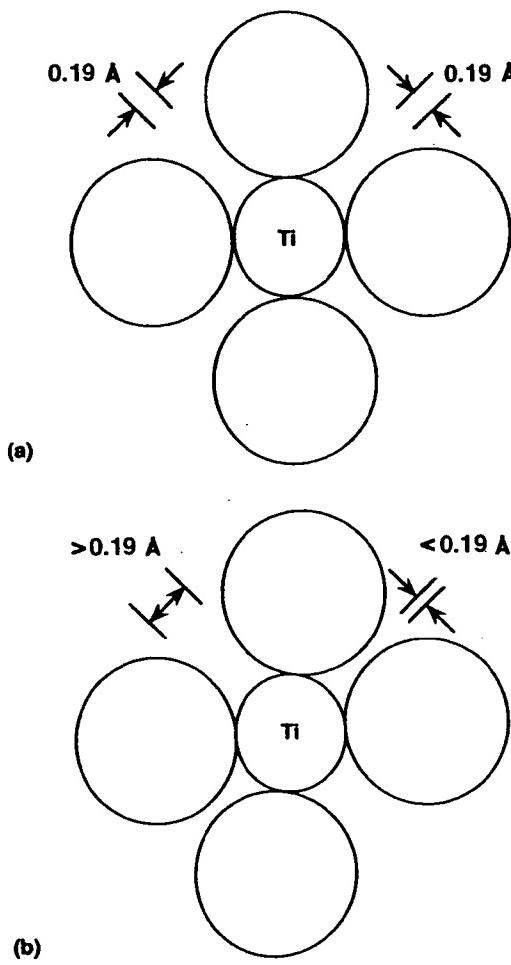
$$\% \text{ ANIS} = \frac{100|b - a|}{\frac{1}{2}(b + a)} = 0.22\%, \quad (7.3)$$

is less than that of most orthorhombic copper oxide superconductors. We see from Fig. 7.5 that in the cubic phase the oxygen atoms in the  $z = 0$  plane are separated by  $0.19 \text{ \AA}$ . The rhombal distortion increases this O-O separation in one direction and decreases it in the other, in the manner indicated in Fig. 7.6a, to produce the Ti nearest-neighbor configuration shown in Fig. 7.6b. This arrangement helps to fit the titanium into its lattice site.

The transformation from tetragonal to orthorhombic is generally of the rhombal type for  $(\text{La}_{1-x}\text{Sr}_x)_2\text{CuO}_4$  and of the rectilinear type for  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ .



**Figure 7.4** Rectangular- (top) and rhombal- (bottom) type distortions of a two-dimensional square unit cell of width  $a$  (Poole *et al.*, 1989).



**Figure 7.6** Shift of the oxygens in the *a*, *b*-plane around the titanium atom of perovskite from the room-temperature tetragonal (and cubic) configuration (a) to the rhombal configuration (b) of its low-temperature orthorhombic structure.

#### D. Planar Representation

Another way of picturing the structure of perovskite is to think of the atoms as forming horizontal planes. If we adopt the notation [E F C] to designate the occupation of the E, F, and C sites, the sketches of perovskite presented in Figs. 7.1 and 7.3 follow the scheme

$$\begin{aligned}
 z = 1 & \quad [\text{TiO}_2^-] \quad \text{Ti at E, O at two F sites} \\
 z = \frac{1}{2} & \quad [\text{O-Ba}] \quad \text{O at E, Ba at C} \\
 z = 0 & \quad [\text{TiO}_2^-] \quad \text{Ti at E, O at two F sites.}
 \end{aligned} \tag{7.4}$$

The planes at the heights  $z = 0$ ,  $\frac{1}{2}$ , and 1 can be labeled using this notation. The

usefulness of this labeling scheme will be clarified in Section V.

This completes our treatment of the structure of perovskite. We encountered many features that we will meet again in the analogous superconductor cases, and established notation that will be useful in describing the structure of the cuprates. However, before proceeding we present details about a cubic and a close-to-cubic perovskite superconductor in the following two sections.

### III. CUBIC BARIUM POTASSIUM BISMUTH OXIDE

The compound



which forms for  $x > 0.25$ , crystallizes in the cubic perovskite structure with  $a = 4.29 \text{ \AA}$  (Cava *et al.*, 1988; Jin *et al.*, 1992; Mattheiss *et al.*, 1988).  $\text{K}^+$  ions replace some of the  $\text{Ba}^{2+}$  ions in the C site, and Bi ions occupy the E sites of Eq. (7.2) (Hinks *et al.*, 1988b; Kwei *et al.*, 1989; Pei *et al.*, 1990; Salem-Sugui *et al.*, 1991; Schneemeyer *et al.*, 1988). Some oxygen sites are vacant, as indicated by  $y$ . Hinks *et al.* (1989) and Pei *et al.* (1990) determined the structural phase diagram (cf. Kuentzler *et al.*, 1991; Zubkus *et al.*, 1991). We should note from Table 7.1 that the potassium (1.33  $\text{\AA}$ ) and barium (1.32  $\text{\AA}$ ) ions are almost the same size, and that  $\text{Bi}^{5+}$  (0.74  $\text{\AA}$ ) is close to  $\text{Ti}^{4+}$  (0.68  $\text{\AA}$ ). Bismuth represents a mixture of the valence states  $\text{Bi}^{3+}$  and  $\text{Bi}^{5+}$  which share the  $\text{Ti}^{4+}$  site in a proportion that depends on  $x$  and  $y$ . The larger size (0.96  $\text{\AA}$ ) of the  $\text{Bi}^{3+}$  ion causes the lattice constant  $a$  to expand 7% beyond its cubic  $\text{BaTiO}_3$  value. Oxygen vacancies help to compensate for the larger size of  $\text{Bi}^{3+}$ .

It is noteworthy that  $\text{Ba}_{1-x}\text{K}_x\text{BiO}_{3-y}$  becomes superconducting at a temperature ( $\approx 40 \text{ K}$  for  $x \approx 0.4$ ) that is higher than the  $T_c$  of all of the *A15* compounds. This compound, which has no copper, has

been widely studied in the quest for clues that would elucidate the mechanism of high-temperature superconductivity. Features of  $\text{Ba}_{1-x}\text{K}_x\text{BiO}_{3-y}$ , such as the fact that it contains a variable valence state ion and utilizes oxygen vacancies to achieve charge compensation, reappear in the high-temperature superconducting compounds.

#### IV. BARIUM LEAD BISMUTH OXIDE

In 1983 Mattheiss and Hamann referred to the 1975 "discovery by Sleight *et al.* of high-temperature superconductivity" in the compound  $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$  in the composition range  $0.05 \leq x \leq 0.3$  with  $T_c$  up to 13 K. Many consider this system, which disproportionates  $2\text{Bi}^{4+} \rightarrow \text{Bi}^{3+} + \text{Bi}^{5+}$  in going from the metallic to the semiconducting state, as a predecessor to the  $\text{LaSrCuO}$  system.

The metallic compound  $\text{BaPbO}_3$  is a cubic perovskite with the relatively large lattice constant (Wyckoff, 1964; cf. Nitta *et al.*, 1965; Shannon and Bierstedt, 1970) listed in Table 7.3. At room temperature semiconducting  $\text{BaBiO}_3$  is monoclinic ( $a \approx b \approx c/\sqrt{2}$ ,  $\beta = 90.17^\circ$ ), but close to orthorhombic (Chaillout *et al.*, 1985; Cox and Sleight, 1976, 1979; cf. Federici *et al.*, 1990; Jeon *et al.*, 1990; Shen *et al.*, 1989). These two compounds form a solid solution series  $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$  involving cubic, tetragonal, orthorhombic, and monoclinic modifications. Superconductivity appears in the tetragonal phase, and the metal-to-insulator transition occurs at the tetragonal-to-orthorhombic phase boundary  $x \approx 0.35$  (Gilbert *et al.*, 1978; Koyama and Ishimaru, 1992; Mattheiss, 1990; Mattheiss and Hamann, 1983; Sleight, 1987; cf. Bansil *et al.*, 1991; Ekino and Akimitsu, 1989a, b; Papaconstantopoulos *et al.*, 1989).

The compound resembles



with its variable Bi valence states, but it differs in not exhibiting superconductivity in the cubic phase.

#### V. PEROVSKITE-TYPE SUPERCONDUCTING STRUCTURES

In their first report on high-temperature superconductors Bednorz and Müller (1986) referred to their samples as "metallic, oxygen-deficient ... perovskite-like mixed-valence copper compounds." Subsequent work has confirmed that the new superconductors do indeed possess these characteristics.

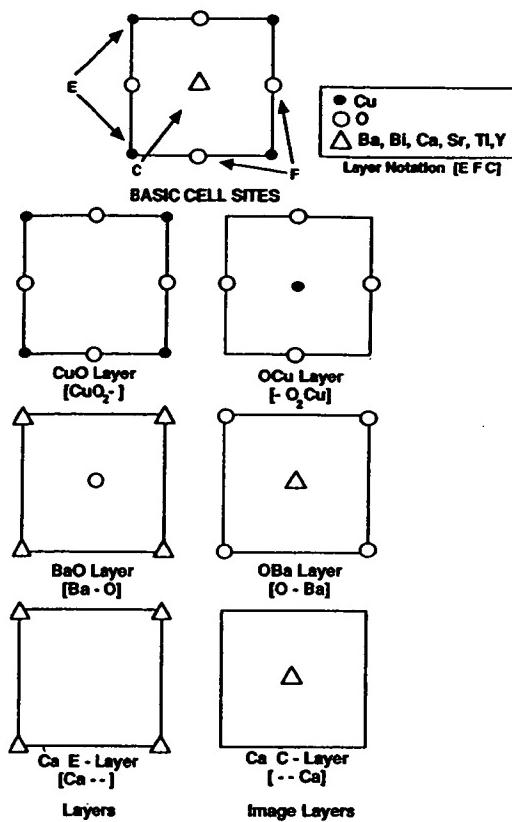
In the oxide superconductors  $\text{Cu}^{2+}$  replaces the  $\text{Ti}^{4+}$  of perovskite, and in most cases the  $\text{TiO}_2$ -perovskite layering is retained as a  $\text{CuO}_2$  layering with two oxygens per copper. Because of this feature of  $\text{CuO}_2$  layers, which is common to all of the high-temperature superconductors, such superconductors exhibit a uniform lattice size in the  $a, b$ -plane, as the data in Table 7.3 demonstrate. The compound  $\text{BaCuO}_3$  does not occur because the  $\text{Cu}^{4+}$  ion does not form, but this valence constraint is overcome by replacement of  $\text{Ba}^{2+}$  by a trivalent ion, such as  $\text{La}^{3+}$  or  $\text{Y}^{3+}$ , by a reduction in the oxygen content, or by both. The result is a set of "layers" containing only one oxygen per cation located between each pair of  $\text{CuO}_2$  layers, or none at all. Each high-temperature superconductor has a unique sequence of layers.

We saw from Eq. (7.2) that each atom in perovskite is located in one of three types of sites. In like manner, each atom at the height  $z$  in a high-temperature superconductor occupies either an Edge (E) site on the edge  $(0, 0, z)$ , a Face (F) site on the midline of a face  $((0, \frac{1}{2}, z) \text{ or } (\frac{1}{2}, 0, z) \text{ or both})$ , or a Centered (C) site centered within the unit cell on the  $z$ -axis  $(\frac{1}{2}, \frac{1}{2}, z)$ . The site occupancy notation [E F C] is used because many cuprates contain a succession of  $[\text{Cu} \text{ O}_2^-]$  and  $[-\text{O}_2 \text{ Cu}]$  layers in which the Cu atom switches between edge and centered sites, with the oxygens

Table 7.3 Crystallographic Characteristics of Oxide Superconducting and Related Compounds<sup>a</sup>

Compound	Symbol	Symm	Type	Enlarg.	units	$a_0(\text{\AA})$	$c_0(\text{\AA})$	$c_0/\text{Cu}$	%Anis	$T_c$ (K)	Comments	Form.
BaTiO <sub>3</sub>	—	C	A	1	1	4.012	4.012	—	0	—	—	$T > 200^\circ\text{C}$
BaTiO <sub>3</sub>	—	T	A	1	1	3.995	4.03	—	0	—	—	$20^\circ\text{C}$
BaTiO <sub>3</sub>	—	O	A	$\sqrt{2}$	2	$4.013\sqrt{2}$	3.990	—	0.23	—	—	$T < 5^\circ\text{C}$
BaPbO <sub>3</sub>	—	C	A	1	1	4.273	4.273	—	0	0.4	—	
BaPb <sub>0.7</sub> Bi <sub>0.3</sub> O <sub>3</sub>	—	T	S	$\sqrt{2}$	4	$4.286\sqrt{2}$	4.304	—	0	12	—	
BaBiO <sub>3</sub>	—	M	A	$\sqrt{2}$	2	$4.355\sqrt{2}$	4.335	—	0.13	—	—	$\beta = 90.17^\circ$
Ba <sub>0.6</sub> K <sub>0.4</sub> BiO <sub>3</sub>	—	C	A	1	1	4.293	4.293	—	0	30	—	
La <sub>2</sub> CuO <sub>4</sub>	0201	T	S	1	2	3.81	13.18	6.59	0	35	Sr, doped	
La <sub>2</sub> CuO <sub>4</sub>	0201	O	S	$\sqrt{2}$	4	$3.960\sqrt{2}$	13.18	6.59	6.85	35	Sr, doped	
YBa <sub>2</sub> Cu <sub>3</sub> O <sub>8</sub>	0213	T	A	1	1	3.902	11.94	3.98	0	—	—	
YBa <sub>2</sub> Cu <sub>3</sub> O <sub>7</sub>	0213	O	A	1	1	3.855	11.68	3.89	1.43	92	—	
Bi <sub>2</sub> Sr <sub>2</sub> CaCu <sub>2</sub> O <sub>8</sub>	2212	T	S	$5\sqrt{2}$	20	$3.81\sqrt{2}$	30.6	7.65	0	84	—	
Bi <sub>2</sub> Sr <sub>2</sub> Ca <sub>2</sub> Cu <sub>3</sub> O <sub>10</sub>	2223	O	S	$5\sqrt{2}$	20	$3.83\sqrt{2}$	37	6.17	0.57	110	—	
Tl <sub>2</sub> Ba <sub>2</sub> CuO <sub>6</sub>	2201	T	S	1	2	3.83	23.24	11.6	0	90	—	
Tl <sub>2</sub> Ba <sub>2</sub> CaCu <sub>2</sub> O <sub>8</sub>	2212	T	S	1	2	3.85	29.4	7.35	0	110	—	
Tl <sub>2</sub> Ba <sub>2</sub> Ca <sub>2</sub> Cu <sub>3</sub> O <sub>10</sub>	2223	T	S	1	2	3.85	35.88	5.98	—	125	—	
TlBa <sub>2</sub> CuO <sub>5</sub>	1201	A	1	1	1	—	9.5	9.5	—	< 17	—	
TlBa <sub>2</sub> CaCu <sub>2</sub> O <sub>7</sub>	1212	A	1	1	1	—	12.7	6.35	—	91	—	
TlBa <sub>2</sub> Ca <sub>2</sub> Cu <sub>3</sub> O <sub>9</sub>	1223	A	1	1	1	—	15.9	5.3	—	116	—	
TlBa <sub>2</sub> Ca <sub>3</sub> Cu <sub>4</sub> O <sub>11</sub>	1234	A	1	1	1	—	19.1	4.78	—	122	—	
TlBa <sub>2</sub> Ca <sub>4</sub> Cu <sub>5</sub> O <sub>13</sub>	1245	A	1	1	1	—	22.3	4.46	—	< 120	—	
HgBa <sub>2</sub> CuO <sub>4</sub>	1201	T	A	1	1	—	—	—	—	95	—	
HgBa <sub>2</sub> CaCu <sub>2</sub> O <sub>6</sub>	1212	T	A	1	1	3.86	12.6	6.3	—	122	—	
HgBa <sub>2</sub> Ca <sub>2</sub> Cu <sub>3</sub> O <sub>8</sub>	1223	T	A	1	1	3.86	17.7	5.2	—	133	—	

<sup>a</sup> Symbol, symmetry (cubic C, tetragonal T, orthorhombic O, monoclinic M); type (aligned A, staggered S); enlargement in  $a$ ,  $b$ -plane (diagonal distortion  $\sqrt{2}$ , superlattice S); formula units per unit cell; lattice parameters ( $a_0$ ,  $c_0$ , and  $c_0$  per Cu ion); % anisotropy; and transition temperature  $T_c$ . For the orthorhombic compounds tabulated values of  $a_0$  are averages of  $a_0$  and  $b_0$ .

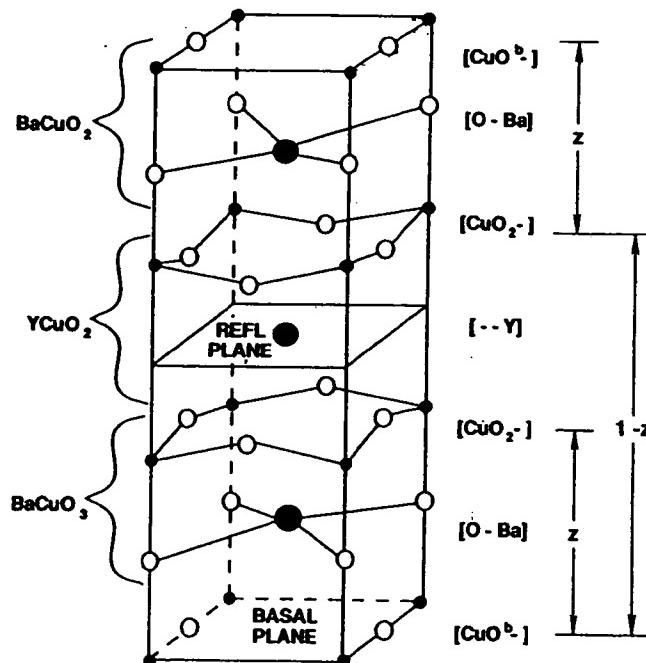


**Figure 7.7** Types of atom positions in the layers of a high-temperature superconductor structure, using the edge, face, center notation [E F C]. Typical site occupancies are given in the upper right (Poole *et al.*, 1989).

remaining at their face positions. Similar alternations in position take place with Ba, O, and Ca layers, as illustrated in Fig. 7.7.

Hauck *et al.* (1991) proposed a classification of superconducting oxide structures in terms of the sequence (1) superconducting layers  $[\text{Cu } \text{O}_2^-]$  and  $[-\text{O}_2 \text{Cu}]$ , (2) insulating layers, such as  $[\text{Y} - -]$  or  $[- - \text{Ca}]$ , and (3) hole-donating layers, such as  $[\text{Cu } \text{O}^b -]$  or  $[\text{Bi} - \text{O}]$ .

The high-temperature superconductor compounds have a horizontal reflection plane ( $\perp$  to  $z$ ) called  $\sigma_h$  at the center of the unit cell and another  $\sigma_h$  reflection plane at the top (and bottom). This means that every plane of atoms in the lower half of the cell at the height  $z$  is duplicated in the upper half at the height  $1-z$ . Such atoms, of course, appear twice in the unit cell, while atoms right on the symmetry planes only occur once since they cannot be reflected. Figure 7.8 shows a  $[\text{Cu } \text{O}_2^-]$  plane at a height  $z$  reflected to the height  $1-z$ . Note how the puckering preserves the reflection symmetry operation. Superconductors that have this reflection plane, but lack end-centering and body-centering op-



**Figure 7.8** Unit cell of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  showing the molecular groupings, reflection plane, and layer types.

erations (see Section VII), are called *aligned* because all of their copper atoms are of one type; either all on the edge ( $0, 0, z$ ) in E positions or all centered ( $\frac{1}{2}, \frac{1}{2}, z$ ) at C sites. In other words, they all lie one above the other on the same vertical lines, as do the Cu ions in Fig. 7.8.

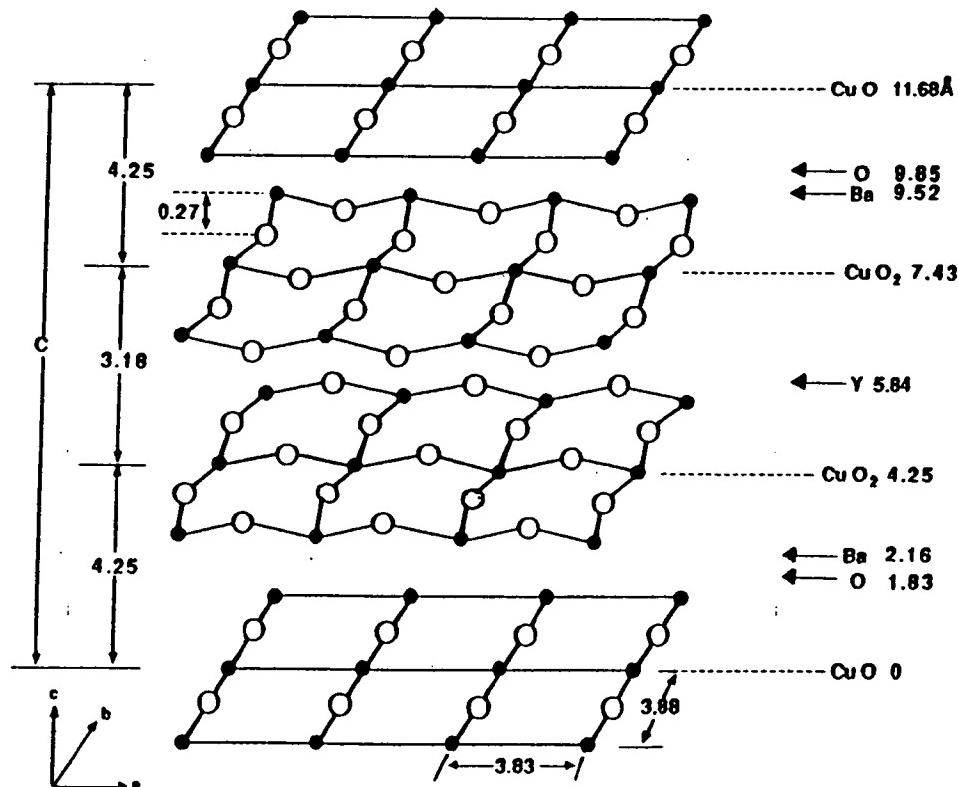
## VI. ALIGNED $\text{YBa}_2\text{Cu}_3\text{O}_7$

The compound  $\text{YBa}_2\text{Cu}_3\text{O}_7$ , sometimes called  $\text{YBaCuO}$  or the 123 compound, in its orthorhombic form is a superconductor below the transition temperature  $T_c \approx 92$  K. Figure 7.8 sketches the locations of the atoms, Fig. 7.9 shows the arrangement of the copper oxide planes, Fig. 7.10 provides more details on the unit cell, and Table 7.4 lists the atom positions and unit cell dimensions (Beno *et al.*, 1987; Capponi *et al.*, 1987; Hazen *et al.*, 1987; Jorgensen *et al.*, 1987; Le Page *et al.*, 1987; Siegrist *et al.*, 1987; Yan and Blanchin,

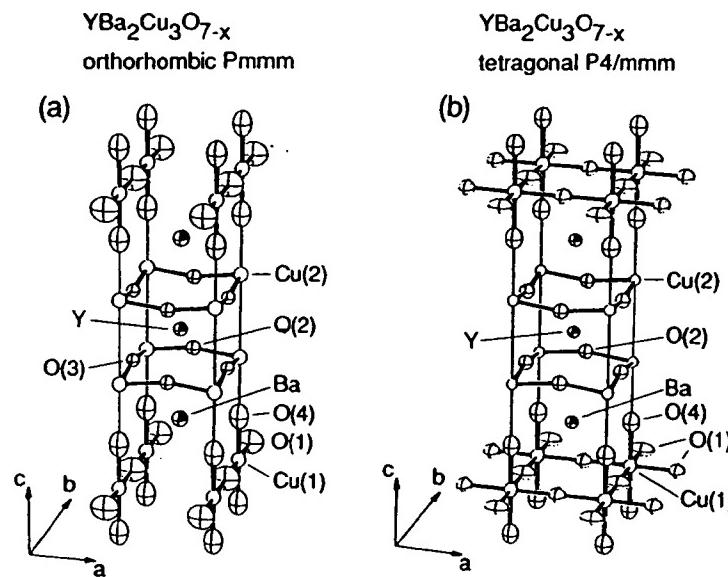
1991; see also Schuller *et al.*, 1987). Considered as a perovskite derivative, it can be looked upon as a stacking of three perovskite units  $\text{BaCuO}_3$ ,  $\text{YCuO}_2$ , and  $\text{BaCuO}_2$ , two of them with a missing oxygen, and this explains why  $c \approx 3a$ . It is, however, more useful to discuss the compound from the viewpoint of its planar structure.

### A. Copper Oxide Planes

We see from Fig. 7.9 that three planes containing Cu and O are sandwiched between two planes containing Ba and O and one plane containing Y. The layering scheme is given on the right side of Fig. 7.8, where the superscript b on O indicates that the oxygen lies along the b-axis, as shown. The atoms are puckered in the two  $[\text{Cu} \text{ O}_2^-]$  planes that have the  $[- \text{---} \text{Y}]$  plane between them. The third copper oxide plane  $[\text{Cu} \text{ O}^{\text{b}}^-]$ , often referred to as



**Figure 7.9** Layering scheme of orthorhombic  $\text{YBa}_2\text{Cu}_3\text{O}_7$ , with the puckering indicated. The layers are perpendicular to the  $c$ -axis (Poole *et al.*, 1988, p. 101).



**Figure 7.10** Sketches of the superconducting orthorhombic (left) and nonsuperconducting tetragonal (right)  $\text{YBaCuO}$  unit cells. Thermal vibration ellipsoids are shown for the atoms. In the tetragonal form the oxygen atoms are randomly dispersed over the basal plane sites (Jorgensen *et al.*, 1987a, b; also see Schuller *et al.*, 1987).

**Table 7.4** Normalized Atom Positions in the  $\text{YBa}_2\text{Cu}_3\text{O}_7$  Orthorhombic Unit Cell (dimensions  $a = 3.83 \text{ \AA}$ ,  $b = 3.88 \text{ \AA}$ , and  $c = 11.68 \text{ \AA}$ )

Layer	Atom	$x$	$y$	$z$
[Cu O <sup>-</sup> ]	Cu(1)	0	0	1
	O(1)	0	$\frac{1}{2}$	1
[O <sup>-</sup> - Ba]	O(4)	0	0	0.8432
	Ba	$\frac{1}{2}$	$\frac{1}{2}$	0.8146
[Cu O <sub>2</sub> <sup>-</sup> ]	Cu(2)	0	0	0.6445
	O(3)	0	$\frac{1}{2}$	0.6219
	O(2)	$\frac{1}{2}$	0	0.6210
[ - - Y ]	Y	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
[Cu O <sub>2</sub> <sup>-</sup> ]	O(2)	$\frac{1}{2}$	0	0.3790
	O(3)	0	$\frac{1}{2}$	0.3781
	Cu(2)	0	0	0.3555
[O <sup>-</sup> - Ba]	Ba	$\frac{1}{2}$	$\frac{1}{2}$	0.1854
	O(4)	0	0	0.1568
	O(1)	0	$\frac{1}{2}$	0
[Cu O <sup>-</sup> ]	Cu(1)	0	0	0

"the chains," consists of  $-\text{Cu}-\text{O}-\text{Cu}-\text{O}-$  chains along the  $b$  axis in lines that are perfectly straight because they are in a horizontal reflection plane  $\sigma_h$ ; where no puckering can occur. Note that, according to the figures, the copper atoms are all stacked one above the other on edge (E) sites, as expected for an aligned-type superconductor. Both the copper oxide planes and the chains contribute to the superconducting properties.

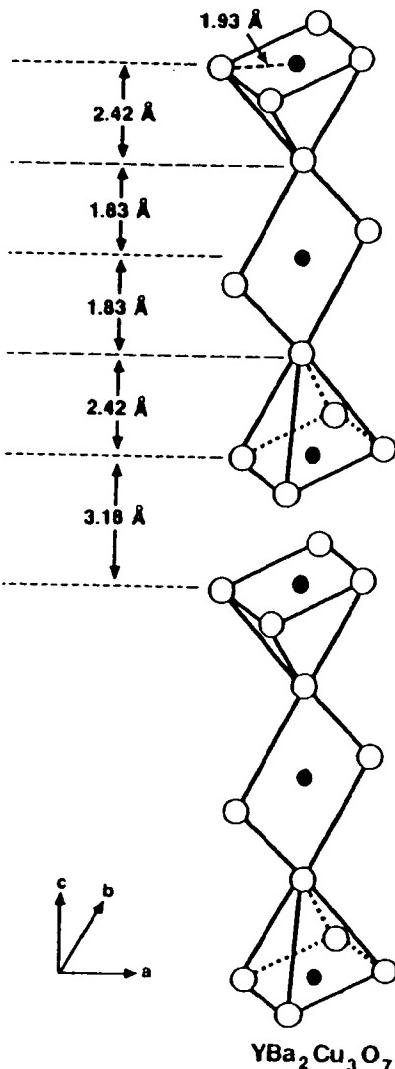
### B. Copper Coordination

Now that we have described the planar structure of  $\text{YBaCuO}$  it will be instructive to examine the local environment of each copper ion. The chain copper ion  $\text{Cu}(1)$  is square planar-coordinated and the two coppers  $\text{Cu}(2)$  and  $\text{Cu}(3)$  in the plane exhibit fivefold pyramidal coordination, as indicated in Fig. 7.11. The ellipsoids at the atom positions of Fig. 7.10 provide a measure of the thermal vibrational motion which the atoms experience, since the amplitudes of the atomic vibrations are indicated by the relative size of each of the ellipsoids.

### C. Stacking Rules

The atoms arrange themselves in the various planes in such a way as to enable them to stack one above the other in an efficient manner, with very little interference from neighboring atoms. Steric effects prevent large atoms such as Ba ( $1.34 \text{ \AA}$ ) and O ( $1.32 \text{ \AA}$ ) from overcrowding a layer or from aligning directly on top of each other in adjacent layers. In many cuprates stacking occurs in accordance with the following two empirical rules:

1. Metal ions occupy either edge or centered sites, and in adjacent layers alternate between E and C sites.
2. Oxygens are found in any type of site, but they occupy only one type in a particular layer, and in adjacent layers they are on different types of sites.



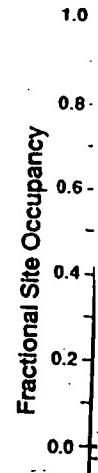
**Figure 7.11** Stacking of pyramid, square-planar, and inverted pyramid groups along the  $c$ -axis of orthorhombic  $\text{YBa}_2\text{Cu}_3\text{O}_7$ , (adapted from Poole *et al.*, 1988, p. 100).

Minor adjustments to make more room can be brought about by puckering or by distorting from tetragonal to orthorhombic.

### D. Crystallographic Phases

The  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  compound comes in tetragonal and orthorhombic varieties, as shown in Fig. 7.10, and it is the latter phase which is ordinarily superconducting. In the tetragonal phase the oxygen sites in the chain layer are about half occupied

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in a random or disordered manner, and in the orthorhombic phase are ordered into  $-\text{Cu}-\text{O}-$  chains along the  $b$  direction. The oxygen vacancy along the  $a$  direction causes the unit cell to compress slightly so that  $a < b$ , and the resulting distortion is of the rectangular type shown in Fig. 7.4a. Increasing the oxygen content so that  $\delta < 0$  causes oxygens to begin occupying the vacant sites along  $a$ . Superlattice ordering of the chains is responsible for the phase that goes superconducting at 60 K.

$\text{YBaCuO}$  is prepared by heating in the 750–900°C range in the presence of various concentrations of oxygen. The compound is tetragonal at the highest temperatures, increases its oxygen content through oxygen uptake and diffusion (Rothman *et al.*, 1991) as the temperature is lowered, and undergoes a second-order phase transition of the order-disorder type at about 700°C to the low-temperature orthorhombic phase, as indicated in Fig. 7.12

(Jorgensen *et al.*, 1987, 1990; Schuller *et al.*, 1987; cf. Beyers and Ahn, 1991; Metzger *et al.*, 1993; Fig. 8). Quenching by rapid cooling from a high temperature can produce at room temperature the tetragonal phase sketched on the right side of Fig. 7.10, and slow annealing favors the orthorhombic phase on the left. Figure 7.12 shows the fractional site occupancy of the oxygens in the chain site  $(0, \frac{1}{2}, 0)$  as a function of the temperature in an oxygen atmosphere. A sample stored under sealed conditions exhibited no degradation in structure or change in  $T_c$  four years later (Sequeira *et al.*, 1992). Ultra-thin films tend to be tetragonal (Streiffer *et al.*, 1991).

### E. Charge Distribution

Information on the charge distributions around atoms in conductors can be obtained from knowledge of their energy bands (see description in Chapter 8). This is most easily accomplished by carrying out a Fourier-type mathematical transformation between the reciprocal  $k_x, k_y, k_z$ -space (cf. Chapter 8, Section II) in which the energy bands are plotted and the coordinate  $x, y, z$ -space, where the charge is distributed. We will present the results obtained for  $\text{YBa}_2\text{Cu}_3\text{O}_7$  in the three vertical symmetry planes ( $x, z$ ,  $y, z$ , and diagonal), all containing the  $z$ -axis through the origin, shown shaded in the unit cell of Fig. 7.13.

Contour plots of the charge density of the valence electrons in these planes are sketched in Fig. 7.14. The high density at the  $\text{Y}^{3+}$  and  $\text{Ba}^{2+}$  sites and the lack of contours around these sites together indicate that these atoms are almost completely ionized, with charges of +3 and +2, respectively. It also shows that these ions are decoupled from the planes above and below. This accounts for the magnetic isolation of the Y site whereby magnetic ions substituted for yttrium do not interfere with the superconducting properties. In contrast, the contours surrounding the Cu and O ions are not characteristic of an

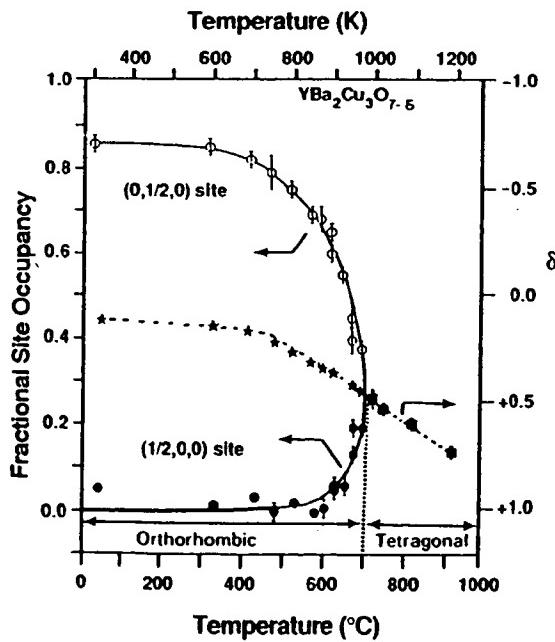
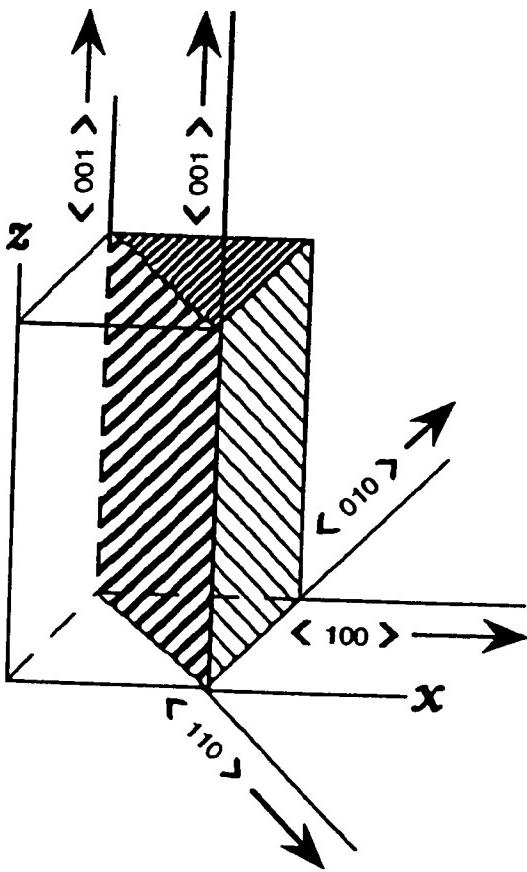
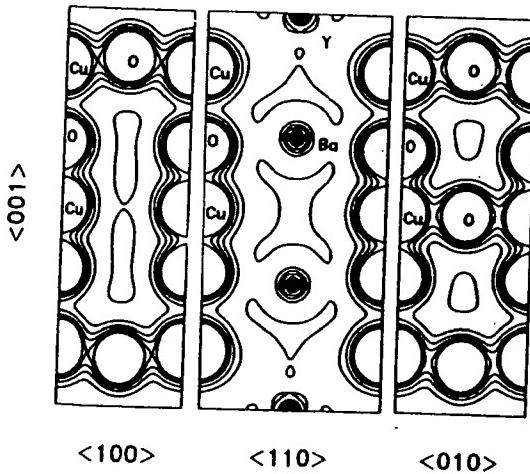


Figure 7.12 Fractional occupancies of the  $(\frac{1}{2}, 0, 0)$  (bottom) and  $(0, \frac{1}{2}, 0)$  (top) sites (scale on left), and the oxygen content parameter  $\delta$  (center, scale on right) for quench temperatures of  $\text{YBaCuO}$  in the range 0–1000°C. The  $\delta$  parameter curve is the average of the two site-occupancy curves (adapted from Jorgensen *et al.*, 1987a; also see Schuller *et al.*, 1987; see also Poole *et al.*, 1988).



**Figure 7.13** Three vertical crystallographic planes ( $x$ ,  $z$ -,  $y$ ,  $z$ -, and diagonal) of a tetragonal unit cell of  $\text{YBa}_2\text{Cu}_3\text{O}_7$ , and standard notation for the four crystallographic directions.



**Figure 7.14** Charge density in the three symmetry planes of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  shown shaded in Fig. 7.13. The  $x$ ,  $z$ , diagonal and the  $y$ ,  $z$  planes are shown from left to right, labeled  $\langle 100 \rangle$ ,  $\langle 110 \rangle$ , and  $\langle 010 \rangle$ , respectively. These results are obtained from band structure calculations, as will be explained in the following chapter (Krakauer and Pickett, 1988).

ordinary ionic compound. The short Cu–O bonds in the planes and chains (1.93–1.96 Å) increase the charge overlap. The least overlap appears in the Cu(2)–O(4) vertical bridging bond, which is also fairly long (2.29 Å). The Cu, O charge contours can be represented by a model that assigns charges of +1.62 and -1.69 to Cu and O, respectively, rather than the values of +2.33 and -2.00 expected for a standard ionic model, where the charge +2.33 is an average of +2, +2, and +3 for the three copper ions. Thus the Cu–O bonds are not completely ionic, but partly covalent.

#### F. $\text{YBaCuO}$ Formula

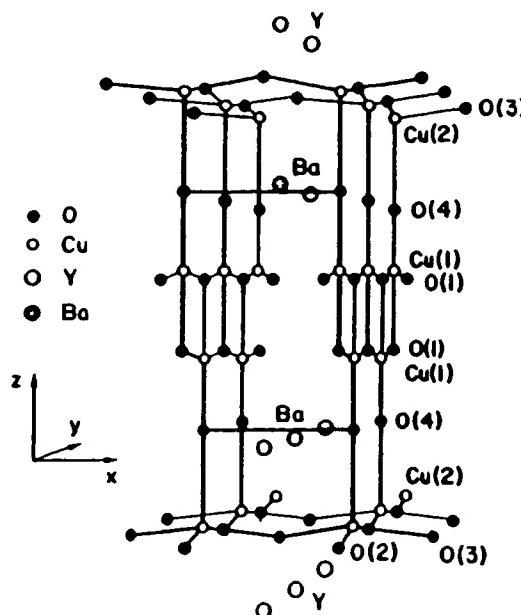
In early work the formula



was used for  $\text{YBaCuO}$  because the prototype triple perovskite  $(\text{YC}\text{uO}_3)(\text{Ba}\text{CuO}_3)_2$  has nine oxygens. Then crystallographers showed that there are eight oxygen sites in the 14-atom  $\text{YBa}_2\text{Cu}_3\text{O}_7$  unit cell, and the formula  $\text{YBa}_2\text{Cu}_3\text{O}_{8-\delta}$  came into widespread use. Finally, structure refinements demonstrated that one of the oxygen sites is systematically vacant in the chain layers, so the more appropriate expression  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  was introduced. It would be preferable to make one more change and use the formula  $\text{Ba}_2\text{YCu}_3\text{O}_{7-\delta}$  to emphasize that Y is analogous to Ca in the bismuth and thallium compounds, but very few workers in the field do this, so we reluctantly adopt the usual “final” notation. In the Bi–Tl compound notation of Section IX, B,  $\text{Ba}_2\text{YCu}_3\text{O}_{7-\delta}$  would be called a 0213 compound. We will follow the usual practice of referring to  $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$  as the 123 compound.

#### G. $\text{YBa}_2\text{Cu}_4\text{O}_8$ and $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_{15}$

These two superconductors are sometimes referred to as the 124 compound and the 247 compound, respectively. They have the property that for each atom at position  $(x, y, z)$  there is another identical atom at

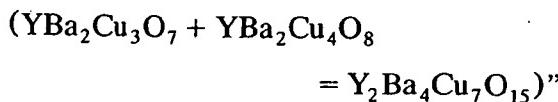


**Figure 7.15** Crystal structure of  $\text{YBa}_2\text{Cu}_4\text{O}_8$  showing how, as a result of the side-centering symmetry operation, the atoms in adjacent Cu–O chains are staggered along the  $y$  direction, with Cu above O and O above Cu (Heyen *et al.*, 1991; modified from Campuzano *et al.*, 1990).

position  $(x, y + \frac{1}{2}, z + \frac{1}{2})$ . In other words, the structure is side centered. This property prevents the stacking rules of Section C from applying.

The chain layer of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  becomes two adjacent chain layers in  $\text{YBa}_2\text{Cu}_4\text{O}_8$ , with the Cu atoms of one chain located directly above or below the O atoms of the other, as shown in Fig. 7.15 (Campuzano *et al.*, 1990; Heyen *et al.*, 1990a, 1991; Iqbal, 1992; Kaldis *et al.*, 1989; Marsh *et al.*, 1988; Morris *et al.*, 1989a). The transition temperature remains in the range from 40 K to 80 K when Y is replaced by various rare earths (Morris *et al.*, 1989). The double chains do not exhibit the variable oxygen stoichiometry of the single ones.

The other side-centered compound,  $\text{Y}_2\text{Ba}_4\text{Cu}_7\text{O}_{15}$ , may be considered according to Torardi, "as an ordered 1:1 intergrowth of the 123 and 124 compounds



(Bordel *et al.*, 1988, Gupta and Gupta, 1993). The 123 single chains can vary in their oxygen content, and superconductivity onsets up to 90 K have been observed. This compound has been synthesized with several rare earths substituted for Y (Morris *et al.*, 1989b).

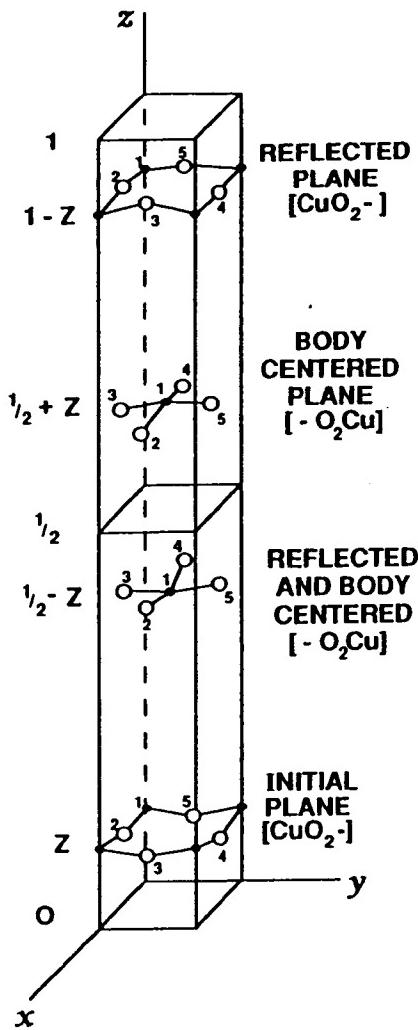
## VII. BODY CENTERING

In Section V we discussed aligned-type superconductor structures that possess a horizontal plane of symmetry. Most high-temperature superconductor structures have, besides this  $\sigma_h$  plane, an additional symmetry operation called body centering whereby for every atom with coordinates  $(x, y, z)$  there is an identical atom with coordinates as determined from the following operation:

$$x \rightarrow x \pm \frac{1}{2}, \quad y \rightarrow y \pm \frac{1}{2}, \quad z \rightarrow z \pm \frac{1}{2} \quad (7.5)$$

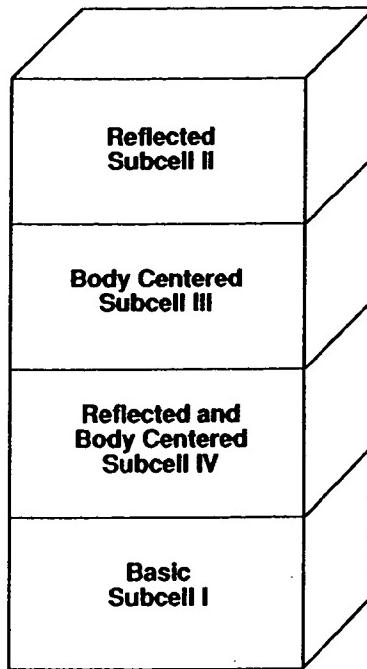
Starting with a plane at the height  $z$  this operation forms what is called an image plane at the height  $z + \frac{1}{2}$  in which the edge atoms become centered, the centered atoms become edge types, and each face atom moves to another face site. In other words, the body-centering operation acting on a plane at the height  $z$  forms a body centered plane, also called an image plane, at the height  $z \pm \frac{1}{2}$ . The signs in these operations are selected so that the generated points and planes remain within the unit cell. Thus if the initial value of  $z$  is greater than  $\frac{1}{2}$ , the minus sign must be selected, viz.,  $z \rightarrow z - \frac{1}{2}$ . Body centering causes half of the Cu–O planes to be  $[\text{Cu } \text{O}_2^-]$ , with the copper atoms at edge sites, and the other half to be  $[- \text{O}_2 \text{Cu}]$ , with the copper atoms at centered sites.

Let us illustrate the symmetry features of a body-centered superconductor by considering the example of  $\text{Tl}_2\text{Ba}_2\text{CaCu}_2\text{O}_8$ . This compound has an initial plane  $[\text{Cu } \text{O}_2^-]$  with the copper and oxygen atoms at the vertical positions  $z = 0.0540$  and 0.0531, respectively, as shown in Fig.



**Figure 7.16** Body-centered tetragonal unit cell containing four puckered  $\text{CuO}_2$  groups showing how the initial group (bottom) is replicated by reflection in the horizontal reflection plane ( $z = \frac{1}{2}$ ), by the body centering operation, and by both.

7.16. For illustrative purposes the figure is drawn for values of  $z$  closer to 0.1. We see from the figure that there is a reflected plane  $[\text{Cu O}_2^-]$  at the height  $1 - z$ , an image (i.e., body centered) plane  $[-\text{O}_2\text{Cu}]$  of the original plane at the height  $\frac{1}{2} + z$ , and an image plane  $[-\text{O}_2\text{Cu}]$  of the reflected plane (i.e., a reflected and body centered plane) at the height  $\frac{1}{2} - z$ . Figure 7.16 illustrates this situation and indicates how the atoms of the initial plane can be transformed into particular atoms in other planes (see Problem 5). Figure 7.17 shows how the configurations of the



**Figure 7.17** Body-centered unit cell divided into four regions by the reflection and body centering operations.

atoms in one-quarter of the unit cell, called the *basic subcell*, or subcell I, determine their configurations in the other three subcells II, III, and IV through the symmetry operations of reflection and body centering.

## VIII. BODY-CENTERED $\text{La}_2\text{CuO}_4$ AND $\text{Nd}_2\text{CuO}_4$

The body-centered compound



has three structural variations in the same crystallographic space group, namely the  $M = \text{La}$  and  $M = \text{Nd}$  types, and a third mixed variety (Xiao *et al.*, 1989). Table 7.5 lists the atom positions of the first two types, and Fig. 7.18 presents sketches of the structures of all three. Each will be discussed in turn.

### A. Unit Cell Generation of $\text{La}_2\text{CuO}_4$ (T Phase)

The structure of the more common  $\text{La}_2\text{CuO}_4$  variety, often called the T phase,

Table 7.5 Atom Positions in the  $\text{La}_2\text{CuO}_4$  and  $\text{Nd}_2\text{CuO}_4$  Structures

$\text{La}_2\text{CuO}_4$ structure						$\text{Nd}_2\text{CuO}_4$ structure					
Layer	Atom	x	y	z		Layer	Atom	x	y	z	
[Cu O <sub>2</sub> -]	O(1)	$\frac{1}{2}$	0	1		[Cu O <sub>2</sub> -]	O(1)	$\frac{1}{2}$	0	1	
	Cu	0	0	1			Cu	0	0	1	
	O(1)	0	$\frac{1}{2}$	1			O(1)	0	$\frac{1}{2}$	1	
	La	$\frac{1}{2}$	$\frac{1}{2}$	0.862	[-- Nd]	Nd	$\frac{1}{2}$	$\frac{1}{2}$	0.862		
[O - La]	O(2)	0	0	0.818	[- O <sub>2</sub> -]	O(3)	0	$\frac{1}{2}$	$\frac{3}{4}$		
	O(2)	$\frac{1}{2}$	$\frac{1}{2}$	0.682		O(3)	$\frac{1}{2}$	0	$\frac{3}{4}$		
[La - O]	La	0	0	0.638	[Nd --]	Nd	0	0	0.638		
	O(1)	$\frac{1}{2}$	0	$\frac{1}{2}$	[- O <sub>2</sub> Cu]	O(1)	$\frac{1}{2}$	0	$\frac{1}{2}$		
	Cu	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		Cu	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$		
	O(1)	0	$\frac{1}{2}$	$\frac{1}{2}$		O(1)	0	$\frac{1}{2}$	$\frac{1}{2}$		
[La - O]	La	0	0	0.362	[Nd --]	Nd	0	0	0.362		
	O(2)	$\frac{1}{2}$	$\frac{1}{2}$	0.318	[- O <sub>2</sub> -]	O(3)	$\frac{1}{2}$	0	$\frac{1}{4}$		
	O(2)	0	0	0.182		O(3)	0	$\frac{1}{2}$	$\frac{1}{4}$		
[O - La]	La	$\frac{1}{2}$	$\frac{1}{2}$	0.138	[-- Nd]	Nd	$\frac{1}{2}$	$\frac{1}{2}$	0.138		
	O(1)	0	$\frac{1}{2}$	0	[Cu O <sub>2</sub> -]	O(1)	0	$\frac{1}{2}$	0		
[Cu O <sub>2</sub> -]	Cu	0	0	0		Cu	0	0	0		
	O(1)	$\frac{1}{2}$	0	0		O(1)	$\frac{1}{2}$	0	0		

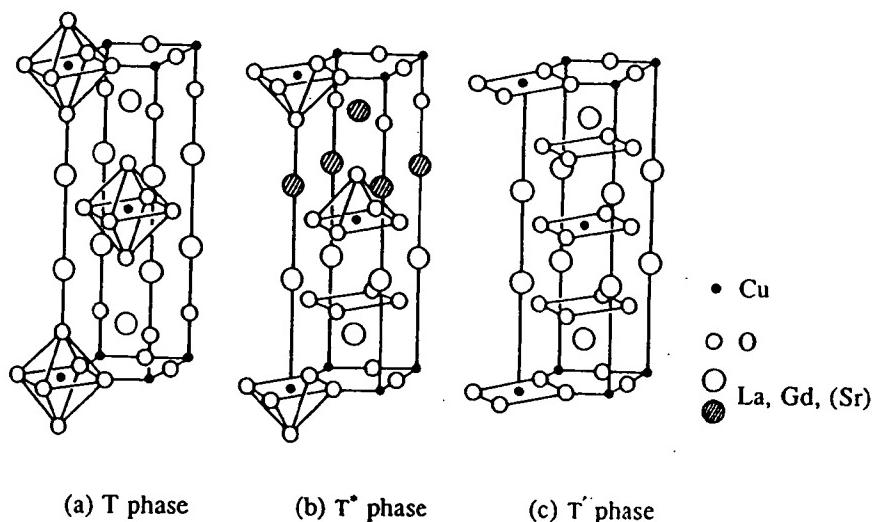


Figure 7.18 (a) Regular unit cell (T phase) associated with hole-type  $(\text{La}_{1-x}\text{Sr}_x)_2\text{CuO}_4$  superconductors, (b) hybrid unit cell ( $\text{T}^*$  phase) of the hole-type  $\text{La}_{2-x-y}\text{R}_y\text{Sr}_x\text{CuO}_4$  superconductors, and (c) alternate unit cell ( $\text{T}'$  phase) associated with electron-type  $(\text{Nd}_{1-x}\text{Ce}_x)_2\text{CuO}_4$  superconductors. The La atoms in the left structure become Nd atoms in the right structure. The upper part of the hybrid cell is T type, and the bottom is T'. The crystallographic space group is the same for all three unit cells (Xiao *et al.*, 1989; see also Oguchi, 1987; Ohbayashi *et al.*, 1987; Poole *et al.*, 1988, p. 83; Tan *et al.*, 1990).

can be pictured as a stacking of  $\text{CuO}_4\text{La}_2$  groups alternately with image (i.e., body centered)  $\text{La}_2\text{O}_4\text{Cu}$  groups along the  $c$  direction, as indicated on the left side of Fig. 7.19 (Cavaet *et al.*, 1987; Kinoshita *et al.*, 1992; Longo and Raccah, 1973; Ohbayashi *et al.*, 1987; Onoda *et al.*, 1987; Zolliker *et al.*, 1990). Another way of visualizing the structure is by generating it from the group  $\text{Cu}_{\frac{1}{2}}\text{O}_2\text{La}$ , comprising the layers  $[\text{O-La}]$  and  $\frac{1}{2}[\text{Cu O}_2^-]$  in subcell I shown on the right side of Fig. 7.19 and also on the left side of Fig. 7.20. (The factor  $\frac{1}{2}$  appears because the  $[\text{Cu O}_2^-]$  layer is shared by two subcells.) Subcell II is formed by reflection from subcell I, and subcells III and IV are formed from I and II via the body-centering operation in the manner of Figs. 7.16 and 7.17. Therefore, subcells I

and II together contain the group  $\text{CuO}_4\text{La}_2$ , and subcells III and IV together contain its image (body centered) counterpart group  $\text{La}_2\text{O}_4\text{Cu}$ . The  $\text{BiSrCaCuO}$  and  $\text{TlBaCaCuO}$  structures to be discussed in Section IX can be generated in the same manner, but with much larger repeat units along the  $c$  direction.

### B. Layering Scheme

The  $\text{La}_2\text{CuO}_4$  layering scheme consists of equally-spaced, flat  $\text{CuO}_2$  layers with their oxygens stacked one above the other, the copper ions alternating between the  $(0, 0, 0)$  and  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$  sites in adjacent layers, as shown in Fig. 7.21. These planes are body-centered images of each other, and are perfectly flat because they are

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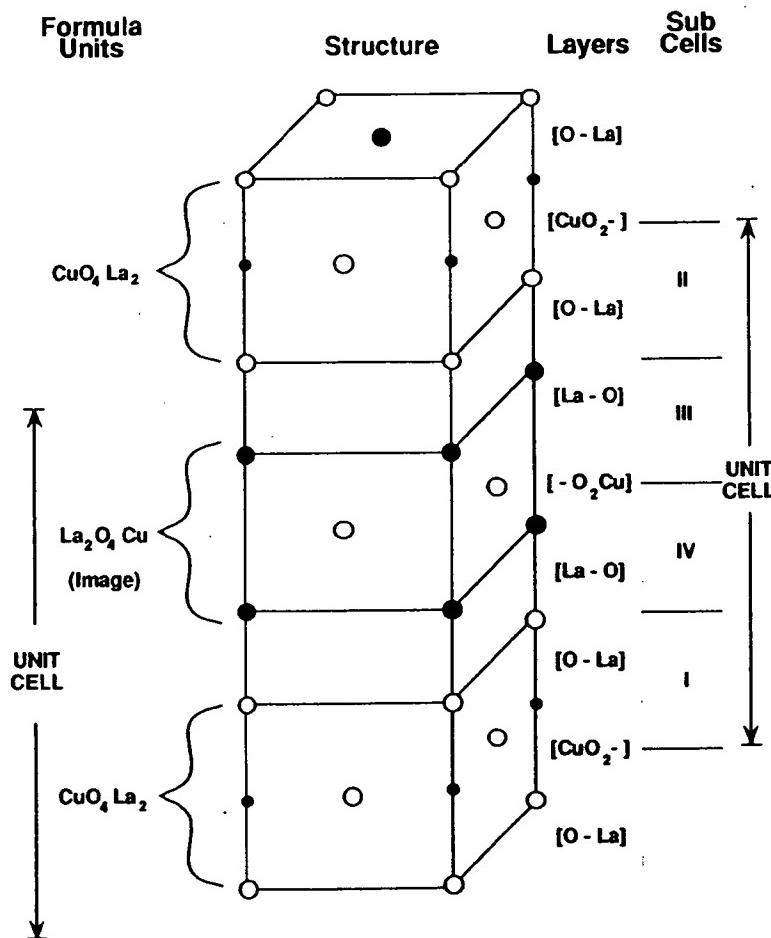


Figure 7.19 Structure of  $\text{La}_2\text{CuO}_4$  (center), showing the formula units (left) and the level labels and subcell types (right). Two choices of unit cell are indicated, the left-side type unit cell based on formula units, and the more common right-side type unit cell based on copper-oxide layers.

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$\text{La}_2\text{CuO}_4$	Sub Cell	$\text{Nd}_2\text{CuO}_4$
$[\text{CuO}_2^-]$	—	$[\text{CuO}_2^-]$
$[\text{O} - \text{La}]$	II	$[- \text{- Nd}]$
$[\text{La} - \text{O}]$	—	$[- \text{O}_2^-]$
$[- \text{O}_2\text{Cu}]$	III	$[\text{Nd} - -]$
$[\text{La} - \text{O}]$	IV	$[\text{Nd} - -]$
$[\text{O} - \text{La}]$	—	$[- \text{O}_2^-]$
$[\text{CuO}_2^-]$	I	$[- \text{- Nd}]$
	—	$[\text{CuO}_2^-]$

Figure 7.20 Layering schemes of the  $\text{La}_2\text{CuO}_4$  (T, left) and  $\text{Nd}_2\text{CuO}_4$  (T', right) structures. The locations of the four subcells of the unit cell are indicated in the center column.

reflection planes. Half of the oxygens, O(1), are in the planes, and the other half, O(2), between the planes. The copper is octahedrally coordinated with oxygen, but the distance 1.9 Å from Cu to O(1) in the  $\text{CuO}_2$  planes is much less than the vertical distance of 2.4 Å from Cu to the apical oxygen O(2), as indicated in Fig. 7.22. The La is ninefold coordinated to four O(1) oxygens, to four O(2) at  $(\frac{1}{2}, \frac{1}{2}, z)$  sites, and to one O(2) at a  $(0, 0, z)$  site.

### C. Charge Distribution

Figure 7.23 shows contours of constant-valence charge density on a logarithmic scale drawn on the back  $x, z$ -plane and on the diagonal plane of the unit cell sketched in Fig. 7.13. These contour plots are obtained from the band structure calculations described in Chapter 8, Section XIV. The high-charge density at the lanthanum site and the low charge density around this site indicate an ionic state

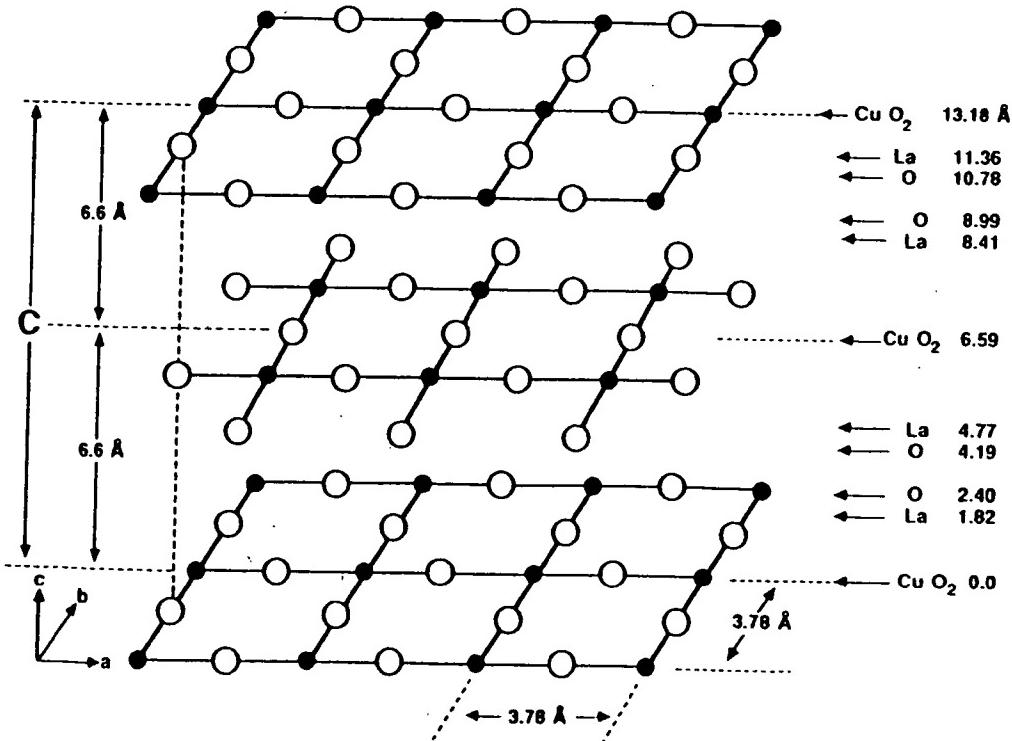
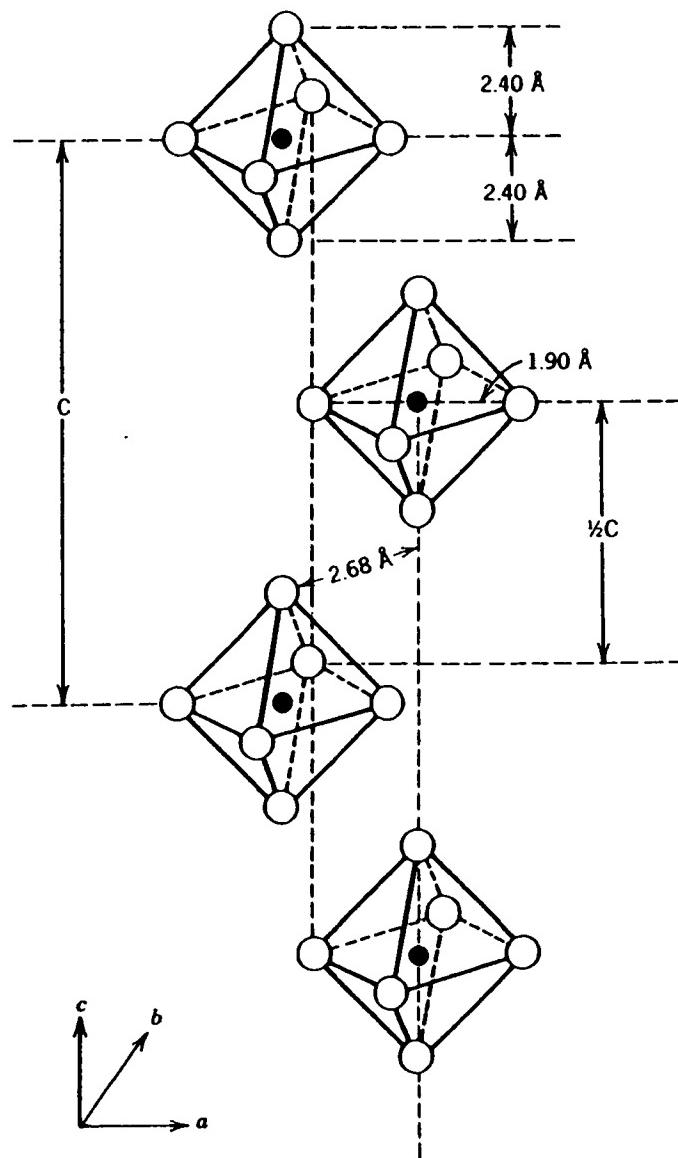


Figure 7.21  $\text{CuO}_2$  layers of the  $\text{La}_2\text{CuO}_4$  structure showing horizontal displacement of Cu atoms in alternate layers. The layers are perpendicular to the  $c$ -axis (Poole *et al.*, 1988, p. 87).



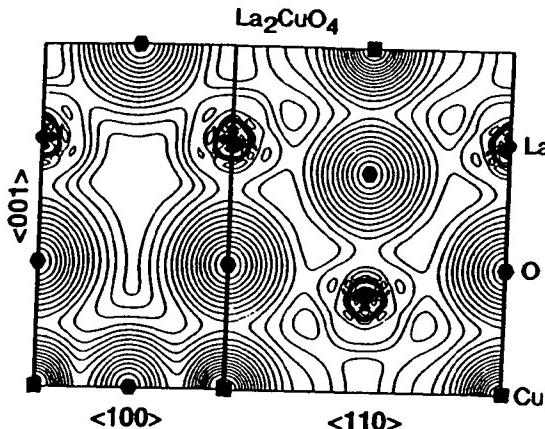
**Figure 7.22** Ordering of axially distorted  $\text{CuO}_6$  octahedra in  $\text{La}_2\text{CuO}_4$  (Poole *et al.*, 1988, p. 88).

$\text{La}^{3+}$ . The charge density changes in a fairly regular manner around the copper and oxygen atoms, both within the  $\text{CuO}_2$  planes and perpendicular to these planes, suggestive of covalency in the Cu–O bonding, as is the case with the  $\text{YBa}_2\text{Cu}_3\text{O}_7$  compound.

#### D. Superconducting Structures

The compound  $\text{La}_2\text{CuO}_4$  is itself an antiferromagnetic insulator and must be doped, generally with an alkaline earth, to exhibit pronounced superconducting prop-

erties. The compounds  $(\text{La}_{1-x}\text{M}_x)_2\text{CuO}_4$ , with 3% to 15% of  $M = \text{Sr}$  or  $\text{Ba}$  replacing  $\text{La}$ , are orthorhombic at low temperatures and low  $M$  contents and are tetragonal otherwise; superconductivity has been found on both sides of this transition. The orthorhombic distortion can be of the rectangular or of the rhomboal type, both of which are sketched in Fig. 7.4. The phase diagram of Fig. 7.24 shows the tetragonal, orthorhombic, superconducting, and anti-ferromagnetically ordered regions for the lanthanum compound (Weber *et al.*, 1989; cf. Goodenough *et al.*, 1993). We see that



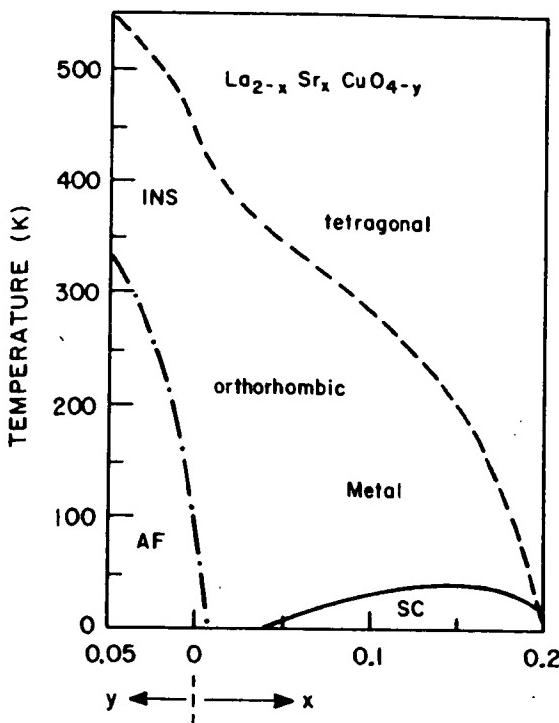
**Figure 7.23** Contour plots of the charge density of  $\text{La}_2\text{CuO}_4$  obtained from band structure calculations. The  $x, z$ -crystallographic plane labeled  $\langle 100 \rangle$  is shown on the left and the diagonal plane labeled  $\langle 110 \rangle$  on the right. The contour spacing is on a logarithmic scale (Pickett, 1989).

the orthorhombic phase is insulating at high temperatures, metallic at low temperatures, and superconducting at very low temperatures. Spin-density waves, to be discussed in Chapter 8, Section XIX, occur in the antiferromagnetic region.

#### E. $\text{Nd}_2\text{CuO}_4$ Compound (T' Phase)

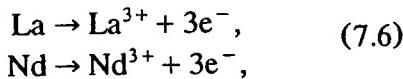
The rarer  $\text{Nd}_2\text{CuO}_4$  structure (Skan-takumar *et al.*, 1989; Sulewski *et al.*, 1990; Tan *et al.*, 1990) given on the right side of Fig. 7.18 and Table 7.5 has all of its atoms in the same positions as the standard  $\text{La}_2\text{CuO}_4$  structure, except for the apical O(2) oxygens in the [O-La] and [La-O] layers, which move to form a  $[-\text{O}_2-]$  layer between  $[-\text{La}-]$  and  $[\text{La}-]$ . These oxygens, now called O(3), have the same  $x, y$  coordinate positions as the O(1) oxygens, and are located exactly between the  $\text{CuO}_2$  planes with  $z = \frac{1}{4}$  or  $\frac{3}{4}$ . We see from Fig. 7.18 that the  $\text{CuO}_6$  octahedra have now lost their apical oxygens, causing Cu to become square planar-coordinated  $\text{CuO}_4$  groups. The Nd is eightfold coordinated to four O(1) and four O(3) atoms, but with slightly different Nd–O distances. The  $\text{CuO}_2$  planes, however, are identical in the two structures. Superconductors with this  $\text{Nd}_2\text{CuO}_4$  structure are of the electron type, in contrast to other high-temperature superconductors, in which the current carriers are holes. In particular, the electron superconductor  $\text{Nd}_{1.85}\text{Ce}_{0.15}\text{CuO}_{4-\delta}$  with  $T_c = 24$  K has been widely studied (Fontcuberta and Fàbrega, 1995, a review chapter; Allen 1990; Alp *et al.*, 1989b; Barlingay *et al.*, 1990; Ekino and Akimitsu, 1989a, b; Lederman *et al.*, 1991; Luke *et al.*, 1990; Lynn *et al.*, 1990; Sugiyama *et al.*, 1991; Tarason *et al.*, 1989a). Other rare earths, such as Pr (Lee *et al.*, 1990) and Sm (Almasan *et al.*, 1992) have replaced Nd.

The difference of structures associated with different signs attached to the current carriers may be understood in terms of the doping process that converts undoped material into a superconductor. Lanthanum and neodymium are both trivalent, and in the undoped compounds they each con-

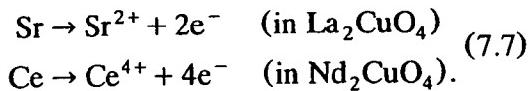


**Figure 7.24** Phase diagram for hole-type  $\text{La}_{2-x}\text{Sr}_x\text{CuO}_{4-y}$ , indicating insulating (INS), antiferromagnetic (AF), and superconducting (SC) regions. Figure VI-6 of Poole *et al.* (1988) shows experimental data along the orthorhombic-to-tetragonal transition line. Spin-density waves (SDW) are found in the AF region (Weber *et al.*, 1989).

tribute three electrons to the nearby oxygens,



to produce  $\text{O}^{2-}$ . To form the superconductors a small amount of La in  $\text{La}_2\text{CuO}_4$  can be replaced with divalent Sr, and some Nd in  $\text{Nd}_2\text{CuO}_4$  can be replaced with tetravalent Ce, corresponding to



Thus, Sr doping decreases the number of electrons to produce hole-type carriers, while Ce doping increases the electron concentration and the conductivity is electron type.

There are also copper-oxide electron superconductors with different structures, such as  $\text{Sr}_{1-x}\text{Nd}_x\text{CuO}_2$  (Smith *et al.*, 1991) and  $\text{TiCa}_{1-x}\text{R}_x\text{Sr}_2\text{Cu}_2\text{O}_{7-\delta}$ , where R is a rare earth (Vijayaraghavan *et al.*, 1989). Electron- and hole-type superconductivity in the cuprates has been compared (Katti and Risbud, 1992; Medina and Regueiro, 1990).

#### F. $\text{La}_{2-x-y}\text{R}_x\text{Sr}_y\text{CuO}_4$ Compounds (T\* Phase)

We have described the T structure of  $\text{La}_2\text{CuO}_4$  and the T' structure of  $\text{Nd}_2\text{CuO}_4$ . The former has O(2) oxygens and the latter O(3) oxygens, which changes the coordinations of the Cu atoms and that of the La and Nd atoms as well. There is a hybrid structure of hole-type superconducting lanthanum cuprates called the T\* structure, illustrated in Fig. 7.18b, in which the upper half of the unit cell is the T type with O(2) oxygens and lower half the T' type with O(3) oxygens. These two varieties of halfcells are stacked alternately along the tetragonal c-axis (Akimitsu *et al.*, 1988; Cheong *et al.*, 1989b; Kwei *et al.*, 1990; Tan *et al.*, 1990). Copper, located in the base of an oxygen pyramid, is fivefold-coordinated  $\text{CuO}_5$ . There are two inequivalent rare earth sites; the ninefold-coordinated site in the T-type halfcell is

preferentially occupied by the larger La and Sr ions, while the smaller rare earths R (i.e., Sm, Eu, Gd, or Tb) prefer the eightfold-coordinated site in the T' half-cell. Tan *et al.* (1991) give a phase diagram for the concentration ranges over which the T and T\* phases are predominant.

#### IX. BODY-CENTERED $\text{BiSrCaCuO}$ AND $\text{TlBaCaCuO}$

Early in 1988 two new superconducting systems with transition temperatures considerably above those attainable with  $\text{YBaCuO}$ , namely the bismuth- and thallium-based materials, were discovered. These compounds have about the same *a* and *b* lattice constants as the yttrium and lanthanum compounds, but with much larger unit cell dimensions along *c*. We will describe their body-centered structures in terms of their layering schemes. In the late 1940s some related compounds were synthesized by the Swedish chemist Bengt Aurivillius (1950, 1951, 1952).

##### A. Layering Scheme

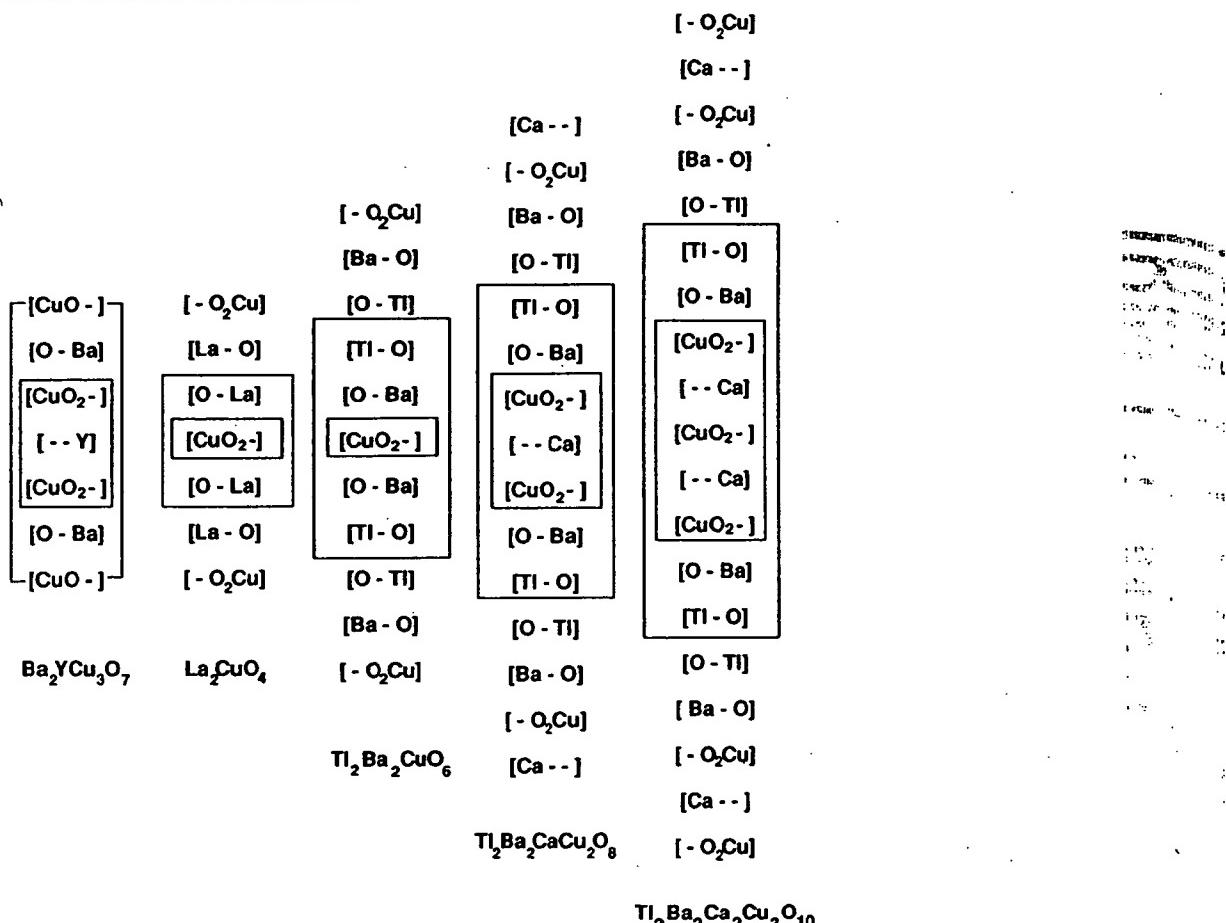
The  $\text{Bi}_2\text{Sr}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{6+2n}$  and  $\text{Tl}_2\text{Ba}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{6+2n}$

compounds, where *n* is an integer, have essentially the same structure and the same layering arrangement (Barry *et al.*, 1989; Siegrist *et al.*, 1988; Torardi *et al.*, 1988a; Yvon and François, 1989), although there are some differences in the detailed atom positions. Here there are groupings of  $\text{CuO}_2$  layers, each separated from the next by Ca layers with no oxygen. The  $\text{CuO}_2$  groupings are bound together by intervening layers of  $\text{BiO}$  and  $\text{SrO}$  for the bismuth compound, and by intervening layers of  $\text{TlO}$  and  $\text{BaO}$  for the thallium compound. Figure 7.25 compares the layering scheme of the  $\text{Tl}_2\text{Ba}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{6+2n}$  compounds with *n* = 0, 1, 2 with those of the lanthanum and yttrium compounds. We also see from the figure that the groupings of  $[\text{CuO}_2]$  planes and  $[-\text{O}_2\text{Cu}]$  image

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**Figure 7.25** Layering schemes of various high-temperature superconductors. The  $\text{CuO}_2$  plane layers are enclosed in small inner boxes, and the layers that make up a formula unit are enclosed in larger boxes. The Bi-Sr compounds  $\text{Bi}_2\text{Sr}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{6+2n}$  have the same layering schemes as their Tl-Ba counterparts shown in this figure.

(i.e., body centered) planes repeat along the  $c$ -axis. It is these copper-oxide layers that are responsible for the superconducting properties.

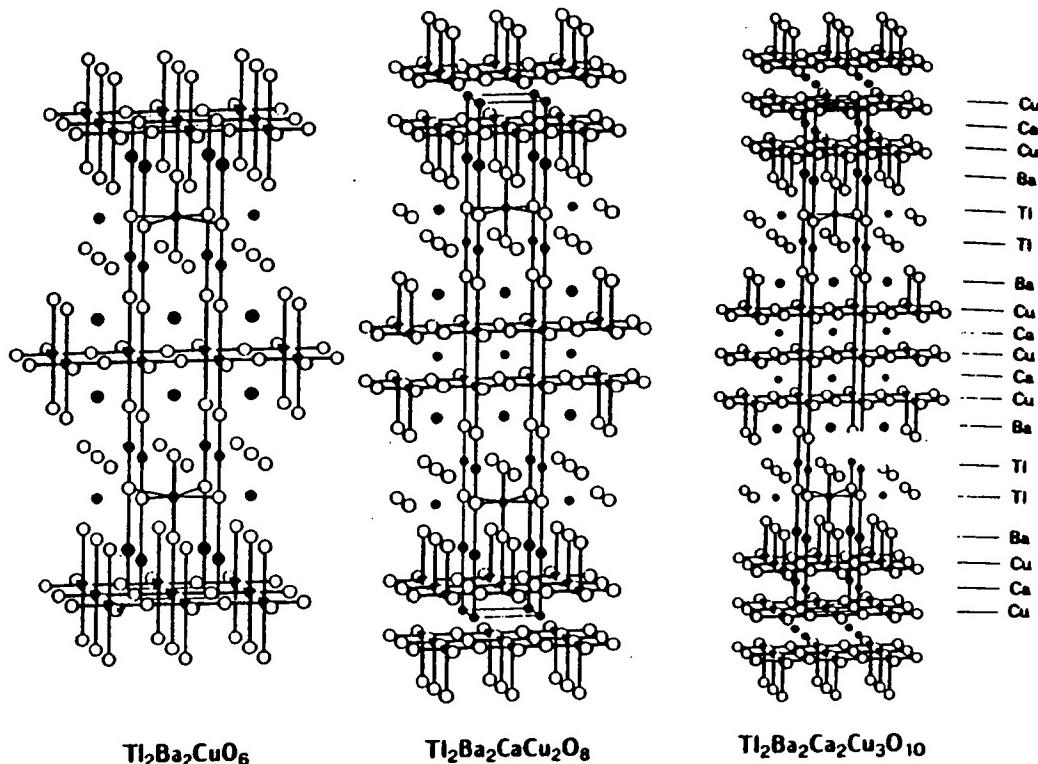
A close examination of this figure shows that the general stacking rules mentioned in Section VI.C for the layering scheme are satisfied, namely metal ions in adjacent layers alternate between edge (E) and centered (C) sites, and adjacent layers never have oxygens on the same types of sites. The horizontal reflection symmetry at the central point of the cell is evident. It is also clear that  $\text{YBa}_2\text{Cu}_3\text{O}_7$  is aligned and that the other four compounds are staggered.

Figure 7.26 (Torardi *et al.*, 1988a) presents a more graphical representation of the information in Fig. 7.25 by showing the

positions of the atoms in their layers. The symmetry and body centering rules are also evident on this figure. Rao (1991) provided sketches for the six compounds  $\text{Tl}_m\text{Ba}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_x$  similar to those in Fig. 7.26 with the compound containing one ( $m = 1$ ) or two thallium layers ( $m = 2$ ), where  $n = 0, 1, 2$ , as in the Torardi *et al.* figure.

## B. Nomenclature

There are always two thalliums and two bariums in the basic formula for  $\text{Tl}_2\text{Ba}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{6+2n}$ , together with  $n$  calciums and  $n + 1$  coppers. The first three members of this series for  $n = 0, 1$ , and 2 are called the 2201, 2212, and 2223 compounds, respectively, and similarly for their



**Figure 7.26** Crystal structures of  $Tl_2Ba_2Ca_nCu_{n+1}O_{6+2n}$  superconducting compounds with  $n = 0, 1, 2$  arranged to display the layering schemes. The  $Bi_2Sr_2Ca_nCu_{n+1}O_{6+2n}$  compounds have the same respective structures (Torardi *et al.*, 1988a).

BiSr analogues  $Bi_2Sr_2Ca_nCu_{n+1}O_{6+2n}$ . Since Y in  $YBa_2Cu_3O_7$  is structurally analogous to Ca in the Tl and Bi compounds, it would be more consistent to write  $Ba_2YC_{u_3}O_7$  for its formula, as noted in Section VI.F. In this spirit  $Bi_2YC_{u_3}O_{7-\delta}$  might be called the 0213 compound, and  $(La_{1-x}M_x)_2CuO_{4-\delta}$  could be called 2001.

### C. Bi-Sr Compounds

Now that the overall structures and interrelationships of the BiSr and TlBa high-temperature superconductors have been made clear in Figs. 7.25 and 7.26 we will comment briefly about each compound. Table 7.3 summarizes the characteristics of these and related compounds.

The first member of the BiSr series, the 2201 compound with  $n = 0$ , has octahedrally coordinated Cu and  $T_c \approx 9$  K (Torardi *et al.*, 1988b). The second mem-

ber,  $Bi_2(Sr,Ca)_3Cu_2O_{8+\delta}$ , is a superconductor with  $T_c \approx 90$  K (Subramanian *et al.*, 1988a; Tarascon *et al.*, 1988b). There are two  $[Cu O_2^-]$  layers separated from each other by the  $[- - Ca]$  layer. The spacing from  $[Cu O_2^-]$  to  $[- - Ca]$  is  $1.66 \text{ \AA}$ , which is less than the corresponding spacing of  $1.99 \text{ \AA}$  between the levels  $[Cu O_2^-]$  and  $[- - Y]$  of  $YBaCuO$ . In both cases the copper ions have a pyramidal oxygen coordination of the type shown in Fig. 7.11. Superlattice structures have been reported along  $a$  and  $b$ , which means that minor modifications of the unit cells repeat approximately every five lattice spacings, as explained in Sect. IX.E. The third member of the series,  $Bi_2Sr_2Ca_2Cu_3O_{10}$ , has three  $CuO_2$  layers separated from each other by  $[- - Ca]$  planes and a higher transition temperature, 110 K, when doped with Pb. The two Cu ions have pyramidal coordination, while the third is square planar.

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indicate the same type of covalency in the Cu–O bonding as with the  $\text{YBa}_2\text{Cu}_3\text{O}_7$  and  $\text{La}_2\text{CuO}_4$  compounds. They also indicate very little bonding between the adjacent [Bi – O] and [O – Bi] layers.

#### D. Tl–Ba Compounds

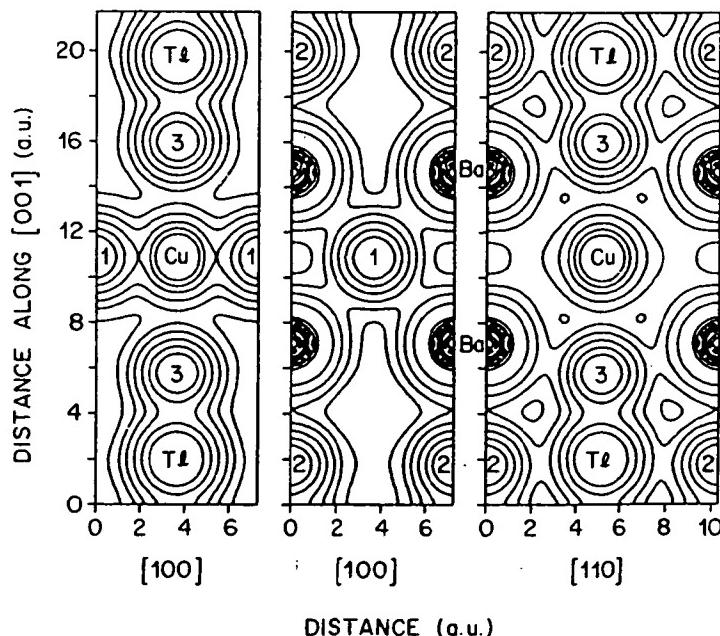
The TlBa compounds



have higher transition temperatures than their bismuth counterparts (Iqbal *et al.*, 1989; Subramanian *et al.*, 1988b; Torardi *et al.*, 1988a). The first member of the series, namely  $\text{Tl}_2\text{Ba}_2\text{CuO}_6$  with  $n = 0$ , has no [– Ca] layer and a relatively low transition temperature of  $\approx 85$  K. The second member ( $n = 1$ ),  $\text{Tl}_2\text{Ba}_2\text{CaCu}_2\text{O}_8$ , called the 2212 compound, with  $T_c = 110$  K,

has the same layering scheme as its Bi counterpart, detailed in Figs. 7.25 and 7.26. The  $[\text{Cu O}_2^-]$  layers are thicker and closer together than the corresponding layers of the bismuth compound (Toby *et al.*, 1990). The third member of the series,  $\text{Tl}_2\text{Ba}_2\text{Ca}_2\text{Cu}_3\text{O}_{10}$ , has three  $[\text{Cu O}_2^-]$  layers separated from each other by [– Ca] planes, and the highest transition temperature, 125 K, of this series of thallium compounds. It has the same copper coordination as its BiSr counterpart. The 2212 and 2223 compounds are tetragonal and belong to the same crystallographic space group as  $\text{La}_2\text{CuO}_4$ .

We see from the charge-density plot of  $\text{Tl}_2\text{Ba}_2\text{CuO}_6$  shown in Fig. 7.27 that  $\text{Ba}^{2+}$  is ionic, Cu exhibits strong covalency, especially in the Cu–O plane, and Tl also appears to have a pronounced covalency. The bonding between the [Tl – O] and [O – Tl] planes is stronger than that between the [Bi – O] and [O – Bi] planes of Bi–Sr.

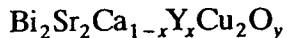


**Figure 7.27** Contours of constant charge density on a logarithmic scale in two high-symmetry crystallographic planes of  $\text{Tl}_2\text{Ba}_2\text{CuO}_6$ . Oxygen atoms O(1), O(2), and O(3) are denoted 1, 2, and 3, respectively. The planar Cu–O1 binding is strongest (Hamann and Mattheiss, 1988; see Pickett, 1989).

### E. Modulated Structures

The x-ray and neutron-diffraction patterns obtained during crystal structure determinations of the bismuth cuprates  $\text{Bi}_2\text{Sr}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{6+2n}$  exhibit weak satellite lines with spacings that do not arise from an integral multiple of the unit cell dimensions. These satellites have modulation periods of 21 Å, 19.6 Å, and 20.8 Å, respectively, for the  $n = 0, 1$ , and 2 compounds (Li *et al.*, 1989). Since the lattice constant  $a = 5.41$  Å ( $b = 5.43$  Å) for all three compounds, this corresponds to a superlattice with unit cell of dimensions  $\approx 3.8a, b, c$ , with the repeat unit along the  $a$  direction equal to  $\approx 3.8a$  for all three compounds. A modulation of  $4.7b$  has also been reported (Kulik *et al.*, 1990). This structural modulation is called incommensurate because the repeat unit is not an integral multiple of  $a$ .

Substitutions dramatically change this modulation. The compound



has a period that decreases from about  $4.8b$  for  $x = 0$  to the commensurate value  $4.0b$  for  $x = 1$  (Inoue *et al.*, 1989; Tamegai *et al.*, 1989). Replacing Cu by a transition metal (Fe, Mn, or Co) produces nonsuperconducting compounds with a structural modulation that is commensurate with the lattice spacing (Tarascon *et al.*, 1989b). A modulation-free bismuth-lead cuprate superconductor has been prepared (Manivannan *et al.*, 1991). Kistenmacher (1989) examined substitution-induced superstructures in  $\text{YBa}_2(\text{Cu}_{1-x}M_x)_3\text{O}_7$ . Superlattices with modulation wavelengths as short as 24 Å have been prepared by employing ultra-thin deposition techniques to interpose insulating planes of  $\text{PrBa}_2\text{Cu}_3\text{O}_7$  between superconducting Cu-O layers of  $\text{YBa}_2\text{Cu}_3\text{O}_7$  (Jakob *et al.*, 1991; Lowndes *et al.*, 1990; Pennycook *et al.*, 1991; Rajagopal and Mahanti, 1991; Triscone *et al.*, 1990). Tanaka and Tsukada (1991) used the Kronig-Penney model (Tanaka and

Tsukada, 1989a,b) to calculate the quasi-particle spectrum of superlattices.

### F. Aligned Tl-Ba Compounds

A series of aligned thallium-based superconducting compounds that have the general formula  $\text{TlBa}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{5+2n}$  with  $n$  varying from 0 to 5 has been reported (Ihara *et al.*, 1988; Rona, 1990). These constitute a series from 1201 to 1245. They have superconducting transition temperatures almost as high as the  $\text{Tl}_2\text{Ba}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{6+2n}$  compounds. Data on these compounds are listed in Table 7.3.

### G. Lead Doping

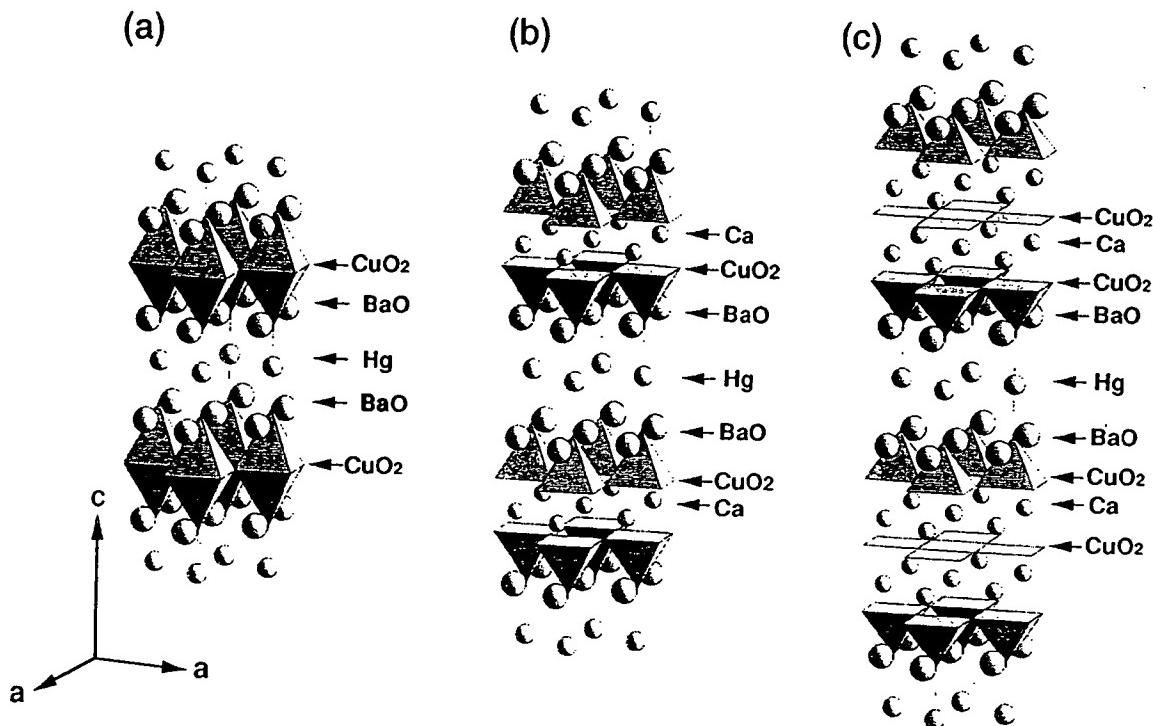
In recent years a great deal of effort has been expended in synthesizing lead-doped superconducting cuprate structures (Itoh and Uchikawa, 1989). Examples involve substituting Pb for Bi (Dou *et al.*, 1989; Zhengping *et al.*, 1990), for Tl (Barry *et al.*, 1989; Mingzhu *et al.*, 1990), or for both Bi and Tl (Iqbal *et al.*, 1990). Different kinds of Pb, Y-containing superconductors have also been prepared (cf. Mattheiss and Hamann, 1989; Ohta and Maekawa, 1990; Tang *et al.*, 1991; Tokiwa *et al.*, 1990, 1991).

## X. ALIGNED HgBaCaCuO

The series of compounds



where  $n$  is an integer, are prototypes for the Hg family of superconductors. The first three members of the family, with  $n = 0, 1, 2$ , are often referred to as Hg-1201, Hg-1212, and Hg-1223, respectively. They have the structures sketched in Fig. 7.28 (Tokiwa-Yamamoto *et al.*, 1993; see also Martin *et al.*, 1994; Putilin *et al.*, 1991). The lattice constants are  $a = 3.86$  Å for all of them, and  $c = 9.5, 12.6$ , and  $15.7$  Å for  $n = 0, 1, 2$ , respectively. The atom positions of the  $n = 1$  compound are listed in Table 7.6 (Hur *et al.*, 1994). The figure is drawn

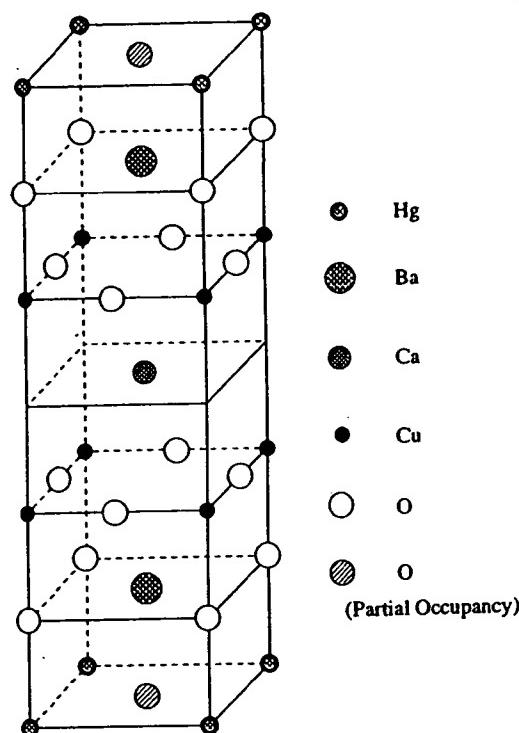


**Figure 7.28** Structural models for the series  $\text{HgBa}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{2n+4}$ . The first three members with  $n = 0, 1, 2$  are shown (parts a, b, and c, respectively) (Tokiwa-Yamamoto *et al.*, 1993).

**Table 7.6** Normalized Atom Positions in the Tetragonal Unit Cell of  $\text{HgBa}_2\text{Ca}_{0.86}\text{Sr}_{0.14}\text{Cu}_2\text{O}_{6+\delta}$

Layer	Atom	x	y	z
[Hg - -]	Hg	0	0	1
	O(3)	$\frac{1}{2}$	$\frac{1}{2}$	1
	O(2)	0	0	0.843
[O - Ba]	Ba	$\frac{1}{2}$	$\frac{1}{2}$	0.778
	Cu	0	0	0.621
	O(1)	0	$\frac{1}{2}$	0.627
[Cu O <sub>2</sub> -]	O(1)	$\frac{1}{2}$	0	0.627
	Ca, Sr	$\frac{1}{2}$	$\frac{1}{2}$	$\frac{1}{2}$
	O(1)	$\frac{1}{2}$	0	0.373
[Cu O <sub>2</sub> -]	O(1)	0	$\frac{1}{2}$	0.373
	Cu	0	0	0.379
	Ba	$\frac{1}{2}$	$\frac{1}{2}$	0.222
[O - Ba]	O(2)	0	0	0.157
	O(3)	$\frac{1}{2}$	$\frac{1}{2}$	0
	Hg	0	0	0

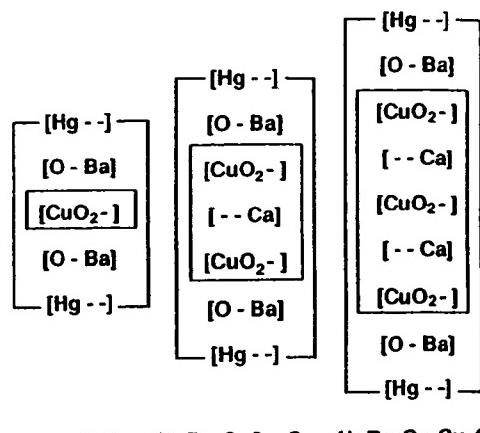
<sup>a</sup> Unit cell dimensions  $a = 3.8584 \text{ \AA}$  and  $c = 12.6646 \text{ \AA}$ , space group is  $P4/mmm$ ,  $D_{4h}^1$ . The Hg site is 91% occupied and the O(3) site is 11% occupied ( $\delta = 0.11$ ). The data are from Hur *et al.* (1994).



**Figure 7.29** Schematic structure of the  $\text{HgBa}_2\text{CaCu}_2\text{O}_{6+\delta}$  compound which is also called Hg-1212 (Meng *et al.*, 1993a).

with mercury located in the middle layer of the unit cell, while the table puts Hg at the origin (000) and Ca in the middle ( $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ ). Figure 7.29 presents the unit cell for the  $n = 1$  compound  $\text{HgBa}_2\text{CaCu}_2\text{O}_{6+\delta}$  drawn with Ca in the middle (Meng *et al.*, 1993a). The symbol  $\delta$  represents a small excess of oxygen located in the center of the top and bottom layers, at positions  $\frac{1}{2} \frac{1}{2} 0$  and  $\frac{1}{2} \frac{1}{2} 1$  which are labeled "partial occupancy" in the figure. If this oxygen were included the level symbol would be  $[\text{Hg} - \text{O}]$  instead of  $[\text{Hg} - -]$ . These Hg compound structures are similar to those of the series  $\text{TlBa}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{2n+4}$  mentioned above in Section IX.F.

We see from Fig. 7.28 that the copper atom of Hg-1201 is in the center of a stretched octahedron with the planar oxygens O(1) at a distance of 1.94 Å, and the apical oxygens O(2) of the  $[\text{O} - \text{Ba}]$  layer much further away (2.78 Å). For  $n = 1$  each copper atom is in the center of the



**Figure 7.30** Layering schemes of three  $\text{HgBa}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{2n+4}$  compounds, using the notation of Fig. 7.25.

base of a tetragonal pyramid, and for  $n = 2$  the additional  $\text{CuO}_2$  layer has Cu atoms which are square planar coordinated. The layering scheme stacking rules of Section VI.C are obeyed by the Hg series of compounds, with metal ions in adjacent layers alternating between edge (E) and centered (C) sites, and oxygen in adjacent layers always at different sites. We see from Table 7.6 that the  $[\text{O} - \text{Ba}]$  layer is strongly puckered and the  $[\text{CuO}_2^-]$  layer is only slightly puckered.

The relationships between the layering scheme of the  $\text{HgBa}_2\text{Ca}_n\text{Cu}_{n+1}\text{O}_{2n+4}$  series of compounds and those of the other cuprates may be seen by comparing the sketch of Fig. 7.30 with that of Fig. 7.25. We see that the  $n = 1$  compound  $\text{HgBa}_2\text{CaCu}_2\text{O}_6$  is quite similar in structure to  $\text{YBa}_2\text{Cu}_3\text{O}_7$  with Ca replacing Y in the center and Hg replacing the chains  $[\text{CuO}_2^-]$ . More surprising is the similarity between the arrangement of the atoms in the unit cell of each



compound and the arrangement of the atoms in the semi-unit cell of the corresponding



compound. They are the same except for the replacement of the [Tl - O] layer by [Hg - -], and the fact that the thallium compounds are body centered and the Hg ones are aligned.

Supercells involving polytypes with ordered stacking sequences of different phases, such as Hg-1212 and Hg-1223, along the *c* direction have been reported. The stoichiometry is often



corresponding to equal numbers of the Hg-1212 and Hg-1223 phases (Phillips, 1993; Schilling *et al.*, 1993, 1994).

Detailed structural data have already been reported on various Hg family compounds such as  $\text{HgBa}_2\text{CuO}_{4+\delta}$  (Putlin *et al.*, 1993) and the  $n=1$  compound with partial Eu substitution for Ca (Putlin *et al.*, 1991). The compound



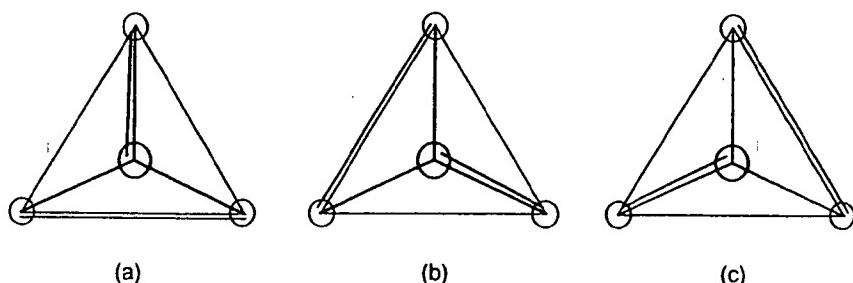
has Hg in the position (0.065, 0, 0), slightly displaced from the origin of the unit cell (Martin *et al.*, 1994). Several researchers have reported synthesis and pretreatment procedures (Adachi *et al.*, 1993; Itoh *et al.*, 1993; Isawa 1994a; Meng, 1993b; Paranthaman, 1994; Paranthaman *et al.*, 1993). Lead doping for Hg has been used to improve the superconducting properties (Iqbal *et al.*, 1994; Isawa *et al.*, 1993; Martin *et al.*, 1994).

## XI. BUCKMINSTERFULLERENES

The compound  $\text{C}_{60}$ , called buckminsterfullerene, or fullerene for short, con-

sists of 60 carbon atoms at the vertices of the dotriacontahedron (32-sided figure) that is sketched in Fig. 3.35 and discussed in Chapter 3, Section XVI. The term fullerene is used here for a wider class of compounds  $\text{C}_n$  with  $n$  carbon atoms, each of whose carbon atoms is bonded to three other carbons to form a closed surface, with the system conjugated such that for every resonant structure each carbon has two single bonds and one double bond. The smallest possible compound of this type is tetrahedral  $\text{C}_4$ , which has the three resonant structures shown in Fig. 7.31. Cubic  $\text{C}_8$  is a fullerene, and we show in Problem 17 that it has nine resonant structures. Icosahedral  $\text{C}_{12}$  is also a fullerene, but octahedral  $\text{C}_6$  and dodecahedral  $\text{C}_{20}$  are not because their carbons are bonded to more than three neighbors. These hypothetical smaller  $\text{C}_n$  compounds have never been synthesized, but the larger ones, such as  $\text{C}_{60}$ ,  $\text{C}_{70}$ ,  $\text{C}_{76}$ ,  $\text{C}_{78}$ , and  $\text{C}_{82}$ , have been made and characterized. Some of them have several forms, with different arrangements of polygons. Clusters of buckminsterfullerenes, such as icosahedral  $(\text{C}_{60})_{13}$ , have also been studied (T. P. Martin *et al.*, 1993).

There are several interesting geometrical characteristics of fullerenes (Chung and Sternberg, 1993). Since each carbon (vertex) joins three bonds (edges) and each edge has two vertices, the number of edges  $E$  in a structure  $\text{C}_n$  is 50% greater than the number of vertices  $V$ . There is a general theorem in topology, called Euler's Theorem, that the number of faces  $F$  of a



**Figure 7.31** The three resonant structures of the (hypothetical) tetrahedral compound  $\text{C}_4$ .

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polyhedron is given by the formula

$$F = E - V + 2. \quad (7.8)$$

In a fullerene  $C_n$  where  $n = V$  three edges meet at each vertex, so we have

$$E = 3V/2, \quad (7.9)$$

$$F = \frac{V}{2} + 2. \quad (7.10)$$

It is shown in Problem 16 that

$$E = \frac{1}{2} \sum_s sF_s \quad (7.11a)$$

$$V = \frac{1}{3} \sum_s sF_s, \quad (7.11b)$$

where  $F_s$  is the number of faces with  $s$  sides, and of course,

$$F = \sum_s F_s. \quad (7.12)$$

Combining Eqs. (7.10)–(7.12) gives the fullerene face formula

$$\sum_s (6 - s)F_s = 12. \quad (7.13)$$

This expression does not place any restrictions on the number of hexagons ( $F_6$ ), but it does severely limit the number of other polyhedra. The two smallest hypothetical fullerenes, the tetrahedron and the cube, have no hexagons, and the larger ones consist of 12 pentagons ( $F_5$ ), from Eq. (7.13), and numerous hexagons. For example, the molecule  $C_{60}$  with  $V = 60$  has 12 pentagons and 20 hexagons. Table 7.7 gives the geometric characteristics of the five Platonic solids, the solids generated by truncating all of their vertices, and several other regular polygons, most of which are fullerenes. The fullerenes of current interest are  $C_{60}$  and larger molecules consisting of 12 pentagons and numerous hexagons, such as  $C_{70}$ ,  $C_{76}$ ,  $C_{78}$ , and  $C_{82}$ . Some have several varieties, such as the isomers of  $C_{78}$  with the symmetries  $C_{2v}$ ,  $D_3$ , and  $D_{3h}$  (Diederich and Whetten, 1992).

The outer diameter of the  $C_{60}$  molecule is 7.10 Å and its van der Waals separation is 2.9 Å, so that the nearest-neighbor distance (effective diameter) in a

Table 7.7 Characteristics of Several Regular Solids<sup>a</sup>

Figure	Vertices	Edges	Faces	Face (polygon) type
Tetrahedron	4	6	4	all equilateral triangles
Octahedron <sup>b</sup>	6	12	8	all equilateral triangles
Cube	8	12	6	all squares
Icosahedron <sup>b</sup>	12	30	20	all equilateral triangles
Dodecahedron (pentagonal)	20	30	12	all regular pentagons
Hexadecahedron	28	42	16	12 pentagons, 4 hexagons
Truncated tetrahedron	12	18	8	4 equilateral triangles, 4 hexagons
Truncated octahedron	24	36	14	6 squares, 8 hexagons
Truncated cube	24	36	14	8 equilateral triangles, 6 octagons
Dotriacontahedron (truncated icosahedron)	60	90	32	12 regular pentagons, 20 hexagons
Truncated dodecahedron	60	90	32	20 equilateral triangles, 12 decagons
Heptatriacontahedron	70	105	37	12 pentagons (2 regular), 25 hexagons
Tetracontahedron	76	114	40	12 pentagons, 28 hexagons
Hentetracontahedron	78	116	41	12 pentagons, 29 hexagons
Dotetracontahedron	84	126	44	12 pentagons, 32 hexagons
Large Fullerene	$n$	$\frac{3}{2}n$	$\frac{1}{2}n + 2$	12 pentagons, $\frac{1}{2}n - 10$ hexagons

<sup>a</sup> The first five solids are the Platonic solids, and the seventh to eleventh are truncations of the Platonic solids. When carbons occupy the vertices all correspond to fullerenes except the octahedron and the icosahedron for which  $3V \neq 2E$ . The smallest compounds in this table have never been synthesized.

<sup>b</sup> Not a fullerene because the vertices have more than three edges.

## XII. SYMMETRIES

solid is 10.0 Å. The bonds shared by a five-membered and a six-membered ring are 1.45 Å long, while those between two adjacent six-membered rings are 1.40 Å long. Above 260 K these molecules form a face centered cubic lattice with lattice constant 14.2 Å; below 260 K it is simple cubic with  $a = 7.10$  Å (Fischer *et al.*, 1991; Kasatani *et al.*, 1993; Troullier and Martins, 1992). When  $C_{60}$  is doped with alkali metals to form a superconductor it crystallizes into a face centered cubic lattice with larger octahedral and smaller tetrahedral holes for the alkalis. The  $C_{60}$  ions are orientationally disordered in the lattice (Gupta and Gupta, 1993).

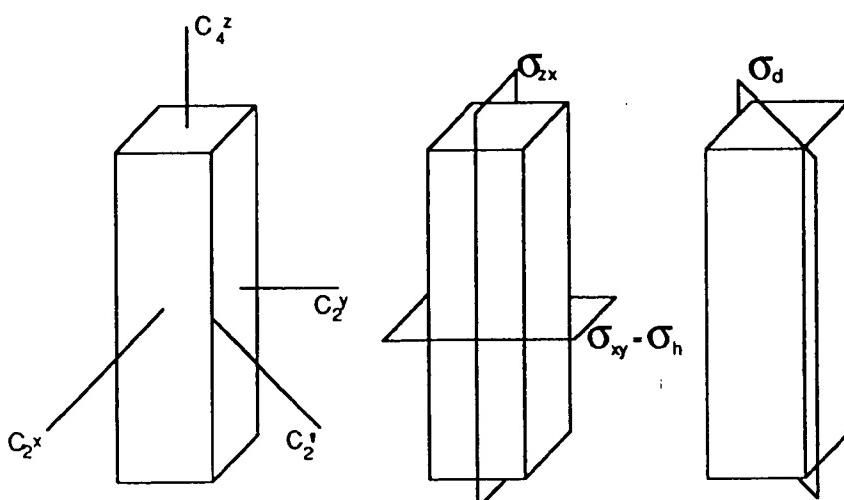
## XII. SYMMETRIES

Earlier in this chapter we mentioned the significance of the horizontal reflection plane  $\sigma_h$  characteristic of the high-temperature superconductors, and noted that most of these superconductors are body centered. In this section we will point out additional symmetries that are present. Table VI-14 of our earlier work (Poole *et al.*, 1988) lists the point symmetries at the sites of the atoms in a number of these compounds.

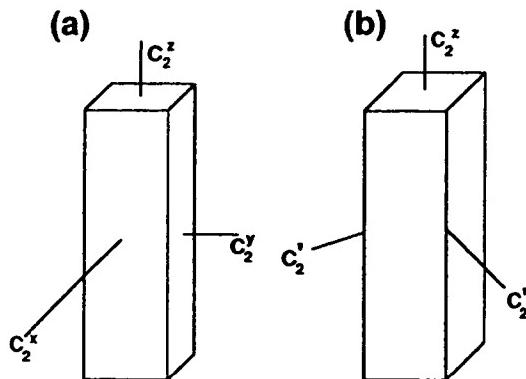
In the notation of group theory the tetragonal structure belongs to the point group  $4/mmm$  (this is the newer international notation for what in the older Schönflies notation was written  $D_{4h}$ ). The unit cell possesses the inversion operation at the center, so when there is an atom at position  $(x, y, z)$ , there will be another identical atom at position  $(-x, -y, -z)$ . The international symbol  $4/mmm$  indicates the presence of a fourfold axis of symmetry  $C_4$  and three mutually perpendicular mirror planes  $m$ . The Schönflies notation  $D_{4h}$  also specifies the fourfold axis,  $h$  signifying a horizontal mirror plane  $\sigma_h$  and  $D$  indicating a dihedral group with vertical mirror planes.

We see from Fig. 7.32 that the  $z$ -axis is a fourfold ( $90^\circ$ ) symmetry axis called  $C_4$ , and that perpendicular to it are twofold ( $180^\circ$ ) symmetry axes along the  $x$  and  $y$  directions, called  $C_2$ , and also along the diagonal directions ( $C'_2$ ) in the midplane. There are two vertical mirror planes  $\sigma_v$ , two diagonal mirror planes  $\sigma_d$  which are also vertical, and a horizontal mirror plane  $\sigma_h$ . Additional symmetry operations that are not shown are a  $180^\circ$  rotation  $C_2^z$  around the  $z$  axis,

$$C_2^z = C_4^z C_4, \quad (7.14)$$



**Figure 7.32** Symmetry operations of the tetragonal unit cell showing a fourfold rotation axis  $C_4$ , three twofold axes  $C_2$ , and reflection planes of the vertical  $\sigma_{zx} = \sigma_v$ , horizontal  $\sigma_{xy} = \sigma_h$ ; and diagonal  $\sigma_d$  types.



**Figure 7.33** Rotational symmetry operations of an orthorhombic unit cell (a) with rectangular distortion, and (b) with rhombal distortion from an originally tetragonal cell.

and the improper fourfold rotation  $S_4^z$  around  $z$  that corresponds to  $C_4^z$  followed by, or preceded by,  $\sigma_h$ ,

$$S_4^z = C_4^z \sigma_h = \sigma_h C_4^z, \quad (7.15)$$

where  $C_4^z$  and  $\sigma_h$  commute.

The orthorhombic structure has  $mmm$ ,  $D_{2h}$  symmetry. We see from Fig. 7.33 that both the rectangular and rhombal unit cells, which correspond to Figs. 7.4a and 7.4b, respectively, have three mutually perpendicular twofold axes, and that they also have three mutually perpendicular mirror planes  $\sigma$ , which are not shown. The two cases differ in having their horizontal axes and vertical planes oriented at  $45^\circ$  to each other.

Cubic structures, being much higher in symmetry, have additional symmetry operations, such as fourfold axes  $C_4^x$ ,  $C_4^y$ , and  $C_4^z$  along each coordinate direction, threefold axes  $C_3$  along each body diagonal, and numerous other mirror planes. These can be easily seen from an examination of Fig. 7.1. Buckyballs belong to the icosohedral group, which has twofold ( $C_2$ ), fivefold ( $C_5$ ), and sixfold ( $C_6$ ) rotation axes, horizontal reflection planes, inversion symmetry, and sixfold ( $S_6$ ) and tenfold ( $S_{10}$ ) improper rotations, for a total of 120 individual symmetry operations in all (Cotton, 1963).

### XIII. CRYSTAL CHEMISTRY

In Chapter 3 we briefly described the structures of some classical superconductors, and in this chapter we provided a more detailed discussion of the structures of the cuprate superconductors. The question arises of how structure is related to the presence of metallic and superconducting properties.

Villars and Phillips (1988; Phillips, 1989a) proposed to explain the combinations of elements in compounds that are favorable for superconductivity at relatively high temperatures by assigning three metallic coordinates to each atom, namely an electron number  $N_e$ , a size  $r$ , and an electronegativity  $X$ . The electron numbers are given in Table 3.1 for most of the elements, with  $N_e = 3$  for all of the rare earths and actinides; several correlations of  $N_e$  with  $T_c$  have already been given in Chapter 3. The sizes and electronegativities were determined empirically from a study of some 3,000 binary intermetallic compounds of types  $AB$ ,  $AB_2$ ,  $AB_3$ , and  $A_2B_5$ . The resulting values for each atom are listed in Fig. 7.34 together with their electron numbers. These values, although arrived at empirically on the basis of the constraint of self-consistency, do have a spectroscopic basis, and thus are called, respectively, *spectroscopic radii* and *spectroscopic electronegativities*.

The metallic coordinates of the atoms can be employed to calculate the three Villars-Phillips (VP) coordinates for each compound, namely (a) average number of valence electrons  $N_v = \langle N_e \rangle_{av}$ , (b) spectroscopic electronegativity difference  $\Delta X$ , and (c) spectroscopic radius difference  $\Delta R$ , where we are using the VP notation. For example, for the compound NbN, with  $T_c = 17.3$  K, we have, using the data from Fig. 7.34,

$$N_v = \frac{1}{2}(4 + 5) = 4.5,$$

$$\Delta R = 2.76 - 0.54 = 2.22, \quad (7.16)$$

$$\Delta X = 2.03 - 2.85 = -0.82.$$

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Na 1 0.89 2.65	Mg 2 1.31 2.03																			
K 1 0.80 3.69	Ca 2 1.17 3.00	Sc 3 1.50 2.75	Ti 4 1.86 2.58	V 5 2.22 2.43	Cr 6 2.00 2.44	Mn 7 2.04 2.22	Fe 8 1.67 2.11	Co 9 1.72 2.02	Ni 10 1.76 2.18	Cu 11 1.08 2.04	Zn 12 1.44 1.88	Ge 3 1.70 1.99	Ge 4 1.99 2.08	As 5 2.27 1.56	Se 6 2.54 1.415	Br 7 2.83 1.285				
Rb 1 0.80 4.10	Sr 2 1.13 3.21	Y 3 1.41 2.94	Zr 4 1.70 2.825	Nb 5 2.03 2.76	Mo 6 1.94 2.72	Tc 7 2.18 2.65	Ru 8 1.97 2.605	Rh 9 1.99 2.52	Pd 10 2.08 2.45	Ag 11 1.07 2.375	Cd 12 1.40 2.215	In 3 1.63 2.05	Sn 4 1.86 1.88	Sb 5 2.14 1.765	Te 6 2.38 1.67	I 7 2.76 1.585				
Cs 1 0.77 4.31	Ba 2 1.08 3.402	La 3 1.35 3.08	Hf 4 1.73 2.91	Ta 5 1.94 2.79	W 6 1.79 2.735	Re 7 2.06 2.64	Os 8 1.85 2.65	Ir 9 1.87 2.62N	Pt 10 1.91 2.70	Au 11 1.19 2.66	Hg 12 1.49 2.41	Tl 3 1.69 2.235	Pb 4 1.92 2.09	Bi 5 2.14 1.997	Po 6 2.40 1.90	At 7 2.64 1.83				
Fr 1 0.70° 4.37°	Ra 2 0.90° 3.53°	Ac 3 1.10° 3.12°																		
Ce 3 1.1° 4.50°	Pr 3 1.1° 4.48°	Nd 3 1.2° 3.99°	Pm 3 1.15° 3.99°	Sm 3 1.2° 4.14°	Eu 3 1.15° 3.94°	Gd 3 1.1° 3.91°	Tb 3 1.2° 3.9°	Dy 3 1.15° 3.67°	Ho 3 1.2° 3.65°	Er 3 1.2° 3.63°	Tm 3 1.2° 3.60°	Yb 3 1.1° 3.59°	Lu 3 1.2° 3.37°							
Th 3 1.3° 4.98°	Pa 3 1.5° 4.96°	U 3 1.7° 4.72°	Np 3 1.3° 4.93°	Pu 3 1.3° 4.91°	Am 3 1.3° 4.89°															

Figure 7.34 Periodic table listing metallic valences (upper right), sizes (center), and electronegativities (bottom) in the box of each element, according to the Villars-Phillips model (Phillips, 1989a, p. 321).

The VP coordinates for the  $A15$  compound  $Ge_3Nb$  with  $T_c = 23.2$  K are calculated as follows:

$$N_v = \frac{1}{4}(4 + 3 \times 5) = 4.75,$$

$$\Delta R = \frac{1}{2}(1.56 - 2.76) = -0.60, \quad (7.17)$$

$$\Delta X = \frac{1}{2}(1.99 - 2.03) = -0.02.$$

The text by Phillips (1989a) tabulates the VP coordinates for more than 60 superconductors with  $T_c > 10$  K and for about 600 additional superconductors with transition temperatures in the range  $1 < T_c < 10$  K.

When the points for the 600 compounds with lower transition temperatures are plotted on a three-dimensional coordinate system with axes  $N_v$ ,  $\Delta X$ , and  $\Delta R$ , they scatter over a large range of values, but when the points for compounds with  $T_c > 10$  K are plotted, they are found to cluster in three regions, called islands, as shown in Fig. 7.35. Island A contains the  $A15$  compounds plus some complex intermetallics, island B consists mainly of the NbN family plus some borides and car-

bides, and island C has closely clustered Chevrel phases, with the high- $T_c$  cuprates on the left. When ternary ferroelectric oxides with Curie temperatures that exceed 500°C are plotted in the same diagram as the superconductors they cluster between the Chevrel group and the cuprates. These ferroelectric oxides are not superconductors, though Phillips (1989a) suggested that doping them with Cu and alkaline earths could produce superconductors with high transition temperatures.

Thus we see that the high transition temperatures of classical superconductors are favored by particular structures and by particular combinations of metallic coordinates for each of these structures. The Villars-Phillips approach provides both structural and atomic criteria for the presence of high  $T_c$ .

We have discussed the Phillips approach to a crystal chemistry explanation of the superconductivity of the cuprates. Other researchers have offered alternate, in some cases somewhat related, approaches to understanding the commonali-

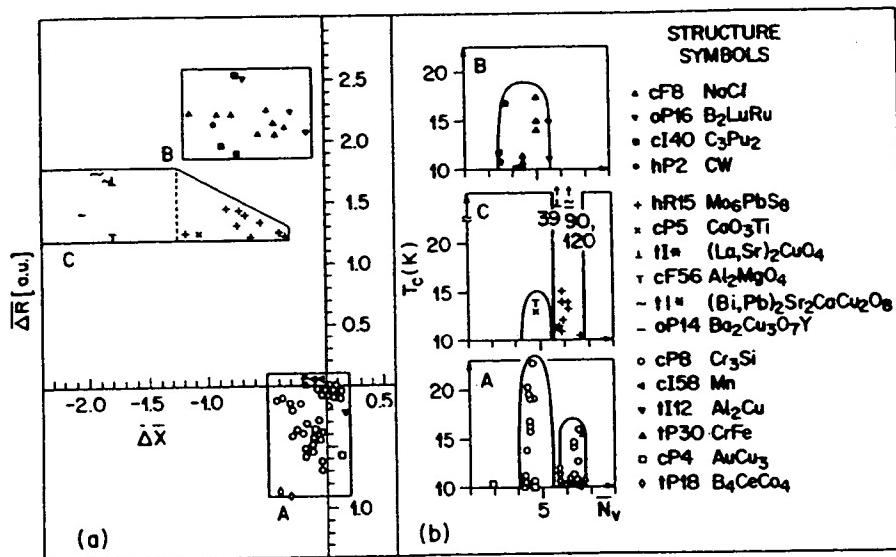


Figure 7.35 Regions in the Villars-Phillips configuration space where superconductivity occurs at relatively high temperatures (Phillips, 1989a, p. 324; Villars and Phillips, 1988).

ties of the various high-temperature and classical superconductors (Adrian, 1992; Schneider, 1992; Tajima and Kitazawa, 1990; Whangbo and Torardi, 1991; Torrance, 1992; Yakhmi and Iyer, 1992; Zhang and Sato, 1993).

#### XIV. COMPARISON WITH CLASSICAL SUPERCONDUCTOR STRUCTURES

Many elements such as copper and lead are face centered cubic, while many other elements, such as niobium, are body centered cubic, with  $a = 3.30 \text{ \AA}$  for Nb. The  $A15$  compounds, such as  $Nb_3Se$ , are (simple) cubic with lattice constant  $a \approx 3.63\sqrt{2}$  and have parallel chains of Nb atoms  $5.14 \text{ \AA}$  apart. Other types of classical superconductors, such as the Laves and Chevrel phases, are cubic or close to cubic. The new oxide superconductors are tetragonal or orthorhombic close to tetragonal, and they all have  $a \approx b \approx 3.85 \text{ \AA}$ , which is somewhat greater than the value for the  $A15$  compounds. The third lattice constant  $c$  varies with the compound, with the values  $13.2 \text{ \AA}$  for  $LaSrCuO$ ,  $11.7 \text{ \AA}$  for  $YBaCuO$ , and  $\approx 23$  to  $36 \text{ \AA}$  for the

$BiSrCaCuO$  and  $TlBaCaCuO$  compounds. These differences occur because the number of copper-oxygen and other planes per unit cell, as well as the spacings between them, vary from compound to compound due to the diverse arrangements of atoms between the layers. Thus relatively high-symmetry crystal structures are characteristic of many superconductors.

#### XV. CONCLUSIONS

Almost all the high-temperature oxide superconductors have point symmetry  $D_{4h}$  ( $a = b$ ) or symmetry close to  $D_{4h}$  ( $a \approx b$ ). These superconductors consist of horizontal layers, each of which contains one positive ion and either zero, one, or two oxygens. The copper ions may be coordinated square planar, pyramidal, or octahedral, with some additional distortion. Copper oxide layers are never adjacent to each other, and equivalent layers are never adjacent. The cations alternate sites vertically, as do the oxygens. The copper oxide layers are either flat or slightly puckered, in contrast to the other metal oxide layers, which are generally far from planar. The highest  $T_c$  compounds have metal layers

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(e.g., Ca) with no oxygens between the copper oxide planes.

## FURTHER READING

The Wyckoff series, *Crystal Structures* (1963, Vol. 1; 1964, Vol. 2; 1965, Vol. 3; 1968, Vol. 4) provides a comprehensive tabulation of crystal structures, but many important classical superconductors such as the *A*15 compounds are not included. The *International Tables for X-Ray Crystallography* (Henry and Lonsdale, 1965, Vol. 1) provide the atom positions and symmetries for all of the crystallographic space groups. The *Strukturbericht* notation, e.g., *A*15 for Nb<sub>3</sub>Ge, is explained in Pearson's compilation (1958).

Details of cuprate crystallographic structures are given by Beyers and Shaw (1989; YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>), Burns and Glazer (1990), Hazen (1990), Poole *et al.* (1988, Chapter 6), Santoro (1990), and Yvon and François (1989). Phillips (1989a) provides an extensive discussion of the crystal chemistry of the cuprates. Our earlier work (Poole *et al.*, 1988, p. 107) lists the site symmetries in perovskite and cuprate structures. Billinge *et al.* (1994) reviewed lattice effects in high temperature superconductors, and Zhu (1994) reviewed structural defects in YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub> .

The microstructure of high temperature superconductors studied by electron microscopy are reviewed by Chen (1990), Gai and Thomas (1992), Gross and Koelle (1994), and Shekhtman (1993). Oxygen stoichiometry in HTSC's is reviewed by Chandrashekhar *et al.*, (1994), Green and Bagley (1990) and by Routbert and Rothman (1995). Electron-doped superconductors are reviewed by Almasan and Maple (1991) and by Fontcuberta and Fàbrega (1995).

The March 1992 special issue of *Accounts of Chemical Research* (Vol. 25, No. 3) is devoted to reviews of buckminsterfullerenes. Two recent books are edited by Billups and Ciofolini (1993) and by Kroto and Walton (1993), and the review by Dresselhaus *et al.* (1994) are devoted to fullerenes. The thallium compounds were reviewed by Hermann and Yakhimi (1993) and the mercury superconductors by Chu (1995).

## PROBLEMS

1. Show that the radius of the octahedral hole in an fcc close-packed lattice of atoms of radius  $r_0$  is equal to  $[\sqrt{2} - 1]r_0$ . What is the radius of the hole if the lattice is formed from oxygen ions?
2. Show that the radius of the tetrahedral hole in an fcc close-packed lattice of atoms of radius  $r_0$  is equal to  $[(3/2)^{1/2}$

$- 1)r_0$ . What is the radius of the hole if the lattice is formed from oxygen ions?

3. The "image perovskite" unit cell is generated from the unit cell of Fig. 7.1 by shifting the origin from the point (0, 0, 0) to the point  $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ . Sketch this "image" cell. Show that the planes of atoms in this cell are the image planes related by the body centering operation to those of the original perovskite. This image cell is the one that usually appears to represent perovskite in solid-state physics texts.
4. Calculate the distance between the yttrium atom and its nearest-neighbor Ba, Cu, and O atoms in the superconductor YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub>.
5. Write down the  $x, y, z$  coordinates for the five numbered atoms in the initial plane of Fig. 7.16. Give the explicit symmetry operations, with the proper choice of sign in Eq. (7.5) for each case, that transform these five atoms to their indicated new positions on the other three planes.
6. Explain how the international and Schönflies symbols, *mmm* and  $D_{2h}$  respectively, are appropriate for designating the point group for the orthorhombic superconductors.
7. What are the symmetry operations of the *A*15 unit cell of Fig. 3.19?
8. The  $D_{2h}$  point group consists of eight symmetry operations that leave an orthorhombic cell unchanged, namely an identity operation *E* that produces no change, three twofold rotations  $C_2^i$  along  $i = x, y, z$ , three mirror reflection planes  $\sigma_{ij}$ , and an inversion *i*. Examples of these symmetry operations are

<i>E</i>	$x \rightarrow x$	$y \rightarrow y$	$z \rightarrow z$
$C_2^x$	$x \rightarrow x$	$y \rightarrow -y$	$z \rightarrow -z$
$\sigma_{xy}$	$x \rightarrow x$	$y \rightarrow y$	$z \rightarrow -z$
<i>i</i>	$x \rightarrow -x$	$y \rightarrow -y$	$z \rightarrow -z$

A group has the property that successive application of two symmetry oper-

ations produces a third. Thus, we have, for example,

$$C_2^x \sigma_{xy} = \sigma_{zx}$$

$$C_2^y C_2^x = C_2^z$$

$$iC_2^y = \sigma_{zx}$$

$$\sigma_{zx} \sigma_{yz} = C_2^z.$$

These results have been entered into the following multiplication table for the  $D_{2h}$  group. Fill in the remainder of the table. Hint: each element of a group appears in each row and each column of the multiplication table once and only once.

$E$	$C_2^x$	$C_2^y$	$C_2^z$	$i$	$\sigma_{xy}$	$\sigma_{yz}$	$\sigma_{zx}$
$E$							
$C_2^x$							$\sigma_{zx}$
$C_2^y$							
$C_2^z$							
$i$							
$\sigma_{xy}$							
$\sigma_{yz}$							
$\sigma_{zx}$							$C_2^z$

- Construct the multiplication table for the  $D_{4h}$  point group which contains the 16 symmetry elements that leave a tetragonal unit cell unchanged. Which pairs of symmetry elements  $A$  and  $B$  do not commute, i.e., such that  $AB \neq BA$ ? Hint: follow the procedures used in Problem 8.
- Draw diagrams analogous to those in Fig. 7.25 for the first two members of the aligned series  $TlBa_2Ca_nCu_{n+1}O_{5+2n}$ , where  $n = 0, 1$ .

- Draw the analogue of Fig. 7.19 for the  $Nd_2CuO_4$  compound, showing the location of all of the Cu and O atoms. How do Figs. 7.21 and 7.22 differ for  $Nd_2CuO_4$ ?
  - Calculate the Villars–Phillips coordinates for the three superconductors  $MoP_3$ ,  $V_3Sn$ , and  $NbTi$ .
  - Select one of the compounds ( $Tl_2Ba_2CuO_6$ ,  $Bi_2Sr_2CaCu_2O_8$ ,  $Bi_2Sr_2Ca_2Cu_3O_{10}$ ,  $Tl_2Ba_2Ca_2Cu_3O_6$ ) and construct a table for it patterned after Tables 7.5 or 7.6.
  - Locate a twofold ( $C_2$ ), fivefold ( $C_5$ ), and sixfold ( $C_6$ ) rotation axis, and also a reflection plane  $\sigma_h$  in the buckyball sketch of Fig. 3.35. How many of each type of operation are there?
  - We can see by examining Fig. 3.35 that a buckyball has inversion symmetry. Identify a sixfold ( $S_6$ ) and tenfold ( $S_{10}$ ) improper rotation axis, where an improper rotation is understood to involve a sequential inversion and a proper rotation. How many  $S_6$  and how many  $S_{10}$  axes are there?
  - Show that the total number of edges  $E$  in a fullerene is given by
- $$E = \frac{1}{2} \sum_s sF_s,$$
- and the number of vortices is
- $$V = \frac{1}{3} \sum_s sF_s,$$
- where  $F_s$  is the number of faces with  $s$  sides.
- Show that the cubic fullerene compound  $C_8$  has nine resonant structures.

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